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PHOTOCHEMICAL OXIDANT MODELING. VOLUME II. DETAILED TECHNICAL REPORT

Robert M. Patterson, et al

GCA Corporation

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PHOTOCHEMICAL OXIDANT MODELING

Volume II -

Detailed Technical Report

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Volume II -
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by

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SECTION I

INTRODUCTION AND SUMMARY

This document reports on a number of somewhat diverse topics, all centered around assessing the oxidant air quality impact of highway project or system modifications arising from the 3-C planning process. The work described here is in support of EPA's goal of providing technical and policy guidance for 109(j) and indirect source reviews of 3-C plans, and for developing air quality maintenance plans for oxidant air quality maintenance areas.

The first section deals with techniques and computer models which are available to calculate mobile source emissions. Comparisons are made of the emission densities estimated by different techniques, and of the various features of the computer models.

Next, a brief summary of a literature survey of the knowledge and theory of oxidant and NO_2 formation is presented. This review is not meant to be exhaustive, but rather to provide enough background for the reader to have a better appreciation of later sections of this report, especially the section which describes the oxidant modeling activities which were undertaken during this project.

In the third section, the oxidant modeling activities which were undertaken for this project are described. This involved a test of Appendix J and a review of three large computer codes — REM (Pacific Environmental Services), DIFKIN (General Research Corporation), and AREAWIDE (Systems Applications Incorporation) — as well as the much simpler

Gifford-Hanna photochemical model. The purpose of this review was to determine which of these models might be used for highway impact evaluation. It was decided to apply the DIFKIN and the Gifford-Hanna models to Denver, based on ease of application, severity of input data requirements, and plausibility of the treatment of atmospheric transport and diffusion and the photochemical reaction processes. The remainder of this section describes the application of these two models and discusses the results.

Completing the report is a "test run" review of 109(j) and indirect source guidelines for Denver, Colorado. During this review it was found that more formal arrangements need to be made to ensure that air quality is considered in transportation planning. It was also found that present guidance does not provide the procedures or methods necessary for deciding whether entire highway systems or component projects are consistent with the air quality goals of state implementation plans. It was determined that the indirect source review procedures do not provide adequate guidance for assessing the oxidant impact of highways.

SECTION II

EMISSIONS MODELS

There are numerous methods for estimating emissions from motor vehicles.[1-8] The basic algorithm is essentially the same for the various methods. By the method given in EPA publication AP-42[1], emission strengths for exhaust hydrocarbons and oxides of nitrogen are calculated by:

$$e_{np} = \sum_{i=n-12}^{n+1} C_{ip}\, d_{ipn}\, m_{in}\, S_{ip} \tag{1}$$

where e_{np} = emissions (grams per vehicle mile) for calendar year n and pollutant p,

c_{ip} = emissions (grams per vehicle mile) for pollutant p for i^{th} model year at low mileage at an average speed of 19.6 miles per hour.

d_{ipn} = emission deterioration factor for the i^{th} model year, calendar year n, and pollutant p for vehicles with emission controls,

m_{in} = weighted annual travel of the i^{th} model year during calendar year n,

and S_{ip} = weighted speed adjustment factor for exhaust emissions of pollutant p for the i^{th} model year.

The weighted speed correction factor, S_{ip}, is in turn computed by the relation:

$$S_{i_m p} = \sum_{j=1}^{k} f_{j_m}\, v_{j_p} \tag{2}$$

with $S_{i_m p}$ = weighted speed adjustment factor for exhaust emissions of pollutant p for the i^{th} model year during calendar year m,

f_{j_m} = the fraction of the total annual vehicle miles traveled at speed j during calendar year m,

v_{jp} = the average speed correction factor for average speed j and pollutant p,

and k = total number of different average speeds.

Evaporative and crankcase hydrocarbon emissions are calculated by:

$$f_n = \sum_{i = n - 12}^{n + 1} h_i \, m_{in} \tag{3}$$

where f_n = combined evaporative and crankcase hydrocarbon emissions for calendar year n,

h_i = combined evaporative and crankcase emission rate (grams per vehicle mile) for the i^{th} model year,

and m_{in} was defined previously.

To calculate actual emissions, e_{np} and f_n must be multiplied by the number of vehicle miles traveled (VMT) for the region of interest during a given time period.

As mentioned earlier, the real differences among vehicle emission models do not arise from the computational methods, but rather from the extent and definition of the input parameters. It can be stated that, in general, newer methods will provide better results because of improved input data, and perhaps because experience provides for improved specification of input parameters. Additional methods[2-5] have been given for computing motor vehicle emissions; almost all use the same basic technique described for AP-42 and all require the same basic data.

A recent technique[6] distinguishes between "hot starts" and "cold starts" in calculating emissions. Cold start data are obtained from the

Federal Test data (AP-42) by assuming a fraction of the test results of total emissions to have occurred during the first 2 minutes or cold start portion of the cycle. This fraction varies with year and is based on General Motors tests results. The grams per mile emissions during the "hot" portion of the test are calculated from the remaining portion of the test sample. The hot emissions are subtracted from the cold emissions to determine the excess emissions attributable exclusively to cold start. The result is a new set of emissions data (grams per mile) for use with VMT data, and a set of "cold start" emissions to be applied where these conditions obtain.

The method has been carried further[7] to define a range of "fractions of a cold start" which increase with an increase in soak time. Starts after a 12-hour soak are considered to be fully cold.

EPA has recently published a supplement[8] revising the internal combustion engine sources portion of AP-42. The new methodology for estimating emissions is quite different from that previously employed and described above due mainly to three factors:

- The new method does not include deterioration factors,
- "Cold start" and "hot start" emissions are included,
- Emissions projections are given in an appendix and not and not listed in the main section dealing with internal combustion engine sources,

The emission factors which are presented in this supplement are based on measurements taken during EPA's annual surveillance programs and cover calendar years 1971 and 1972. Deterioration is accounted for implicitly in the emission factors for the year of measurement. For example, emission factors are presented as X grams per kilometer of exhaust hydrocarbons for a 1969 model year vehicle in calendar year 1972.

Other changes in the method of estimating motor vehicle emissions can best be described by examining the new algorithm used to compute emissions. For light duty vehicles (automobiles) and light duty trucks this is:

$$e_{npstw} = \sum_{i=n-12}^{n} c_{ipn}\, m_{in}\, v_{ips}\, z_{ipt}\, r_{iptw} \tag{4}$$

where e_{npstw} = Composite emission factor in g/km (g/mi) for calendar year n, pollutant p, average speed s, ambient temperature t, and percent cold operation w.

= The FTP (1975 Federal Test Procedure) mean emission factor for the i^{th} model year light duty vehicles during calendar year n and for pollutant p,

m_{in} = The fraction of annual travel by the i^{th} model year light duty vehicles during calendar year n,

v_{ips} = The speed correction factor for the i^{th} model year light duty vehicles for pollutant p and average speed s,

z_{ipt} = The temperature correction factor for the i^{th} model year light duty vehicles for pollutant p and ambient temperature t,

r_{iptw} = The hot/cold vehicle operation correction factor for the i^{th} model year light duty vehicles for pollutant p, ambient temperature, t, and present cold operation w.

The discussion of these variables applies to automobiles and light trucks except where noted.

FTP EMISSION FACTOR (c_{ipn})

These data are divided by geographic area into: low altitude (non-California), high altitude, and California only. The tabulated values are applicable to calendar years 1971 and 1972 (only 1972 for trucks). California emission factors are presented separately since California vehicles have been, in the case of several model years, subject to emission standards which differ from those standards applicable to vehicles under the Federal emission control program. For those model year California vehicles which did not have separate emission standards, the national emission factors are assumed to apply in California as well. Emissions at high altitude are differentiated from those at low altitude to account for the effect that altitude has on air-fuel ratios and concomitant emissions. The tabulated values are applicable to calendar years 1971 and 1972 (only 1972 for trucks) for each model year.

FRACTION OF ANNUAL TRAVEL BY MODEL YEAR (m_i)

No significant change has occurred from previous emission estimation methods.

SPEED CORRECTION FACTORS (v_{ips})

Speed correction factors enable the "adjustment" of FTP emission factors to account for differences in average route speed. Since the implicit average route speed of the FTP is 19.6 miles per hour (31.6 kph), estimates of emissions at higher or lower average speeds require this correction.

It is important to note the difference between "average route speed" and "steady speed." Average route speed is trip-related. It is based on a composite of the driving modes (idle, cruise, acceleration, deceleration) encountered in, for example, a typical home-to-work trip. Steady speed is highway facility-oriented. For instance, a group of vehicles traveling over an uncongested freeway link (volume/capacity of, say, 0.1) might be traveling at a steady speed of about 55 mph (89 kph). Note, however, that steady speeds, even at the link level, are unlikely to occur where resistance to flow occurs (unsynchronized traffic signaling, congested flow, etc.)

Previously, the limited data available for correcting for average speed were presented graphically. Recent research has resulted in revised speed relationships by model year.[6] To facilitate the presentation, the data are given as equations of the form

$$v_{ips} = \exp\ (A + Bs + Cs^2) \qquad (5)$$

where s is the speed in miles per hour.

The values of the coefficients A, B, and C apply only for the range of the data, from 24 to 72 kilometers per hour (15 to 45 miles per hour). Since there is a need, in some situations, to estimate emissions at very low average speeds, correction factors have been developed for this purpose for 8 and 16 kph (5 and 10 mph).

TEMPERATURE CORRECTION FACTOR (z_{ipt})

The 1975 FTP requires that emissions measurements be made within the limits of a relatively narrow temperature band (68^o to 86^oF). Such a band facilitates uniform testing in laboratories without requiring extreme ranges of temperature control. Present emission factors for motor vehicles are based on data from the standard Federal test (assumed to be at 75^oF). The correction factors are expressed in equational form and can be applied between 20^oF and 80^oF. For temperatures outside this range, the appropriate endpoint correction factor is applied.

HOT/COLD VEHICLE OPERATION CORRECTION FACTOR (r_{iptw})

The 1975 FTP measures emissions over three types of driving: a cold transient phase (representative of vehicle start-up after a long engine off period), a hot transient phase (representative of vehicle start-up after a short engine-off period), and a stabilized phase (representative of warmed-up vehicle operation). The weighting factors used in the 1975 FTP are 20 percent, 27 percent, and 53 percent of total miles (time) in each of the three phases respectively. Thus, when the 1975 FTP emission factors are applied to a given region for the purpose of accessing air quality, this can be viewed as if 20 percent of the light duty vehicles in the area of interest are operating in a cold condition, 27 percent are operating in a hot start-up condition, and 53 percent are operating in a hot stabilized condition. For noncatalyst vehicles (all pre 1975 model year vehicles), emissions in the two hot phases are essentially equivalent on a gram/kilometer (grams/mile) basis. Therefore, the 1975 FTP emission factor represents 20 percent cold operation and 80 percent hot operation.

There are many situations where these particular weighting factors may be inappropriate. For example, light duty vehicle operation in the center city may have a much higher percentage of cold operation during the afternoon peak when work-to-home trips are at a maximum and vehicles have been soaking for 8 hours. The hot/cold vehicle operation correction factor allows the cold operation phase to range from 0 percent to 100 percent of total light duty vehicle operations. This correction factor is a function of the percent of cold operation, w, and the ambient temperature, t. The correction factor is:

$$r_{iptw} = \frac{w + (100-w)f(t)}{20 + 80\ f(t)} \qquad (6)$$

where f(t) is a function of temperature presented in AP-42, Supplement No. 5.

The new methodology also allows for calculating evaporative emissions of hydrocarbons and idle emissions of hydrocarbons, nitrogen oxides, and carbon monoxide.

Emissions from light duty, diesel-powered vehicles are calculated as before, except that the emission factors are given for pre-1973 model years. Projection to future years is given as an appendix.

Emissions from heavy-duty gasoline vehicles are calculated by

$$e_{nps} = \sum_{i = n - 12}^{n} c_{ipn} m_{in} v_{ips} \qquad (7)$$

where the factors were defined previously. For heavy-duty diesel-powered vehicles the model year distribution is omitted:

$$e_{nps} = \sum_{i = n - 12}^{n} c_{ipn} v_{ips} \qquad (8)$$

Values for c_{ipn} are based on tests of vehicles on-the-road over the San Antonic Road Route (SARR). The SARR, located in San Antonio, Texas, is 7.24 miles long and includes freeway, arterial and local/collector highway segments. Since the SARR is an actual road route, the average speed varies depending on traffic conditions at the time of the test. However, the average speed tends to be around 29 kph (18 mph) with about 20 percent of the time spent at idle. The test procedure emission factor is composed entirely of warmed-up vehicle operation. Based on a preliminary analysis of vehicle operation data, HDV operation is primarily (about 95 percent) warmed up.

Of course, it is quite necessary to estimate motor vehicle emissions beyond calendar year 1972, and this capability is provided in an appendix to the revised AP-42. This is done purposely to separate the analytical results of EPA's surveillance testing program from what are acknowledged to be "best guesses" of future emission factors. There are several reasons for this separation. First, current legislation allows for limited time extensions for achieving the statutory motor vehicle emission standards. Secondly, Congressional action changing the time table for achieving these standards and/or changing their levels is likely in the future. Thirdly, new data on catalyst-equipped (1975 automobiles) are becoming available. The methods presented in the appendix for estimating emissions are similar to those described above.

There is a final source of data which might prove useful, especially for estimating emissions from higher speed, highway traffic. This is the Modal Analysis Model[9] developed for EPA. This model predicts emissions from a single vehicle or an ensemble of vehicles for a user-specified age distribution over any desired driving sequence within the range of the applicability of the model. The key point for highway traffic is that the model can predict emissions which reflect a constant cruise speed, not an "average route speed" which might include stops and starts. With proper resources, the model could even be used to estimate average emissions for a given urban area based on the typical driving cycle for that area instead of on the Federal Test Procedure.

REFERENCES

1. Compilation of Air Pollutant Emission Factors. EPA Report AP-42 (Second Edition). April 1973.

2. Special Area Analysis (SAPOLLUT Model), U.S. DOT. August 1973.

3. Kircher, David S. and Donald P. Armstrong. An Interim Report on Motor Vehicle Emission Estimation. EPA-450/2-73-003. October 1973.

4. Wolsko, T. D., M. T. Matthies, and R. E. Wendell. Transportation Air Pollution Emissions Handbook. Argonne National Laboratory Report ANL/ES-15. July 1972.

5. Sauter, G. C. and W. R. Ott. A Computer Program for Projections of Vehicular Pollutant Emissions in Urban Areas, JAPCA, 24:54. No. 1 January 1974.

6. Wendell, R. E., J. E. Norco, and K. G. Groke. Emission Prediction and Control Strategy: Evaluation of Pollution from Transportation Systems, JAPCA, 23:91. No. 2. February 1973.

7. Cirillo, R. R., J. E. Norco, and T. D. Wolsko. The Effect of Cold Start on Motor Vehicle Emissions and Resultant Air Quality. Paper 74-127, 67th Annual Meeting, Air Pollution Control Association. Denver. 1974.

8. Supplement No. 5 for Compilation of Air Pollutant Emission Factors. EPA Report AP-42 (Second Edition). Unedited copy. April 1975.

9. Automobile Exhaust Emission Modal Analysis Model. EPA Report EPA-460/3-74-005. January 1974.

SECTION III

SUMMARY OF KNOWLEDGE AND THEORY OF OXIDANT AND NO_2 FORMATION

OXIDANT AND OXIDES OF NITROGEN FORMATION

Fossil fuels are composed of hydrocarbons, combustion of which produces carbon dioxide and water. But since combustion is usually less than 100 percent efficient, the exhaust gases contain unburned fuel which enters the atmosphere. Oxides of nitrogen - in particular, nitric oxide (NO) and nitrogen dioxide (NO_2) - are formed under high-temperature conditions from the combination of atmospheric nitrogen and oxygen. From these inputs of hydrocarbons and oxides of nitrogen to the atmosphere, a complex system of reactions occurs resulting in the formation of oxidants and other products.[1,2]

The series of reactions by which oxidants are formed have been studied to determine the relationship between the precursors and the products.[1,2] Nitric oxide is the primary product formed under high temperature conditions, with only a small amount of NO_2 being formed. NO combines with oxygen to form NO_2:

$$2\ NO + O_2 \rightarrow 2\ NO_2 \qquad (1)$$

Nitrogen dioxide absorbs ultraviolet light from sunlight (photolysis) and the following reactions result:

$$NO_2 \xrightarrow{uv} NO + O \qquad (2)$$

$$O_2 + O \rightarrow O_3 \qquad (3)$$

There are several possible results of the above. The ozone (O_3) may react with nitric oxide, thus reversing the above reactions and completing the nitrogen dioxide photolytic cycle:

$$O_3 + NO \rightarrow NO_2 + O_2 \qquad (4)$$

Alternatively, the oxygen atom or the ozone may react with a hydrocarbon molecule, forming an oxidized hydrocarbon.

The oxidant found in the largest quantity in polluted atmospheres is ozone. Nitric oxide acts as an ozone regulator by reacting with it to form nitrogen dioxide and oxygen (Equation (4)). Ozone does not begin to accumulate in the atmosphere and result in the high ozone concentrations frequently seen until nitric oxide has virtually disappeared. Hydrocarbons interact with the nitrogen dioxide photolytic cycle, leading to the disappearance of nitric oxide and to the accumulation of ozone and hydrocarbon oxidation products.[2] The varying reactivity of different hydrocarbons affects the rate of formation and the amounts of oxidant. In general, the saturated hydrocarbons are the least reactive.

Meteorological variables affect the nitrogen dioxide photolytic cycle and the formation of oxidants.[1,2] The intensity and wavelength of light are important in the photolysis of NO_2. Photolysis is most likely to occur when the light wavelength is between 3000 and 3700A. Light of strong intensity increases the rate of photolysis, so the formation of oxidants is affected when light intensity is affected by such factors as altitude, season or a hazy atmosphere. Temperature also influences the rate of reaction - higher temperatures increase the probability that an endothermic reaction will occur. Therefore, factors which affect temperature (season, time of day) will affect the formation of oxidant. The concentration of precursors and products and thus the rate of formation and the amount of oxidants are influenced by meteorological conditions - wind speed and direction, pressure systems, inversions, and mixing depth. Other variables which affect oxidants formation are topography, the number and distribution of sources, and rates of emission of the precursors.

Oxidants are also formed naturally in any area where the atmosphere contains NO_x and reactive hydrocarbons. Ozone is also formed in the atmosphere by electrical discharge or at high altitudes by solar radiation.

TEMPORAL AND SPATIAL CHARACTERISTICS

Because the nitrogen dioxide photolytic cycle and the formation of oxidants are influenced by meteorological variables, the concentrations of the precursors and products show certain temporal and spatial patterns.[1-5]

In urban areas, a weekday diurnal pattern of NO, NO_2, and O_3 has been noticed - Figure 1 shows a typical pattern for a day in Los Angeles. Levels of all three pollutants are low during the night. Nitric oxide and hydrocarbons are emitted in large quantities by morning rush hour traffic. Nitric oxide is oxidized to nitrogen dioxide (Equation (2)) and since hydrocarbons are present, the reaction tends not to be reversed (Equations (3 and 4)). During the late morning, as the intensity of sunlight increases, nitrogen dioxide reacts with hydrocarbons, and ozone and other oxidants begin to accumulate. Peak ozone levels occur usually from 11:00 a.m. to 2:00 p.m. and are determined by the rate of destruction of ozone.[4] Atmospheric instability, decreased traffic, and the formation of oxidants all help to decrease precursor concentrations during the middle of the day. Afternoon rush hour traffic contributes more NO and hydrocarbons, thus increasing NO_x concentrations. But since the intensity of sunlight has decreased, little ozone is formed and, in fact, the accumulated ozone tends to be destroyed by nitric oxide, returning to low nighttime levels. Figure 1 shows the time relationships of the pollutant peaks. The early afternoon ozone peak is noticeably lower on cloudy days and on sunny days when the wind speed increases. The nitric oxide and nitrogen dioxide peaks are also noticeably lower on windy days. The concentrations of all the pollutants are higher when the mixing depth is less.[1]

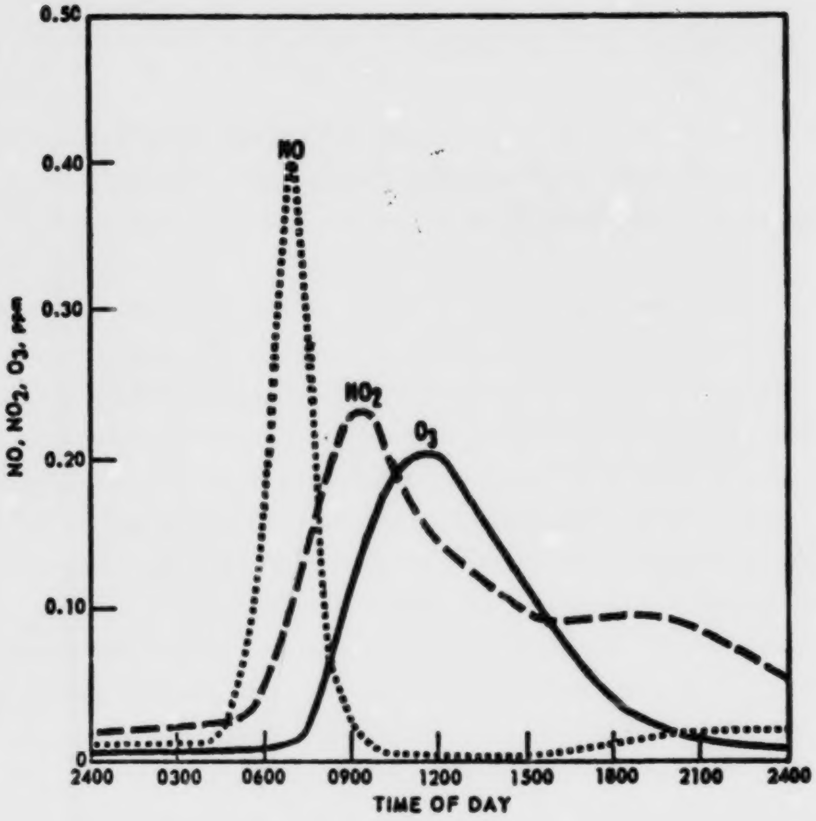


Figure 1. Average daily 1-hour concentrations of selected pollutants in Los Angeles, California, July 19, 1965[2]

The diurnal patterns of NO, NO_2, and O_3 on weekends appear to be different from weekdays,[2,3,5,6] Figure 2 shows, using Chicago as a typical example, how the average emission input levels of NO drop considerably due to decreased traffic. But Figure 3 shows that ozone may be even higher on the weekends, as it was in New York City, though the emissions of precursors have been reduced. It has been hypothesized that this is due to less NO available to regulate ozone levels, to a different NO_2/NO ratio, or to persistence of partially reacted hydrocarbons.[3] This suggests that a reduction in traffic volume with a corresponding decrease in NO and hydrocarbon emissions may actually increase oxidant concentrations.[5,6]

The concentrations of NO, NO_2 and O_3 also show seasonal patterns.[1,2,4] Nitric oxide mean concentrations are higher during late fall and winter when there is less atmospheric mixing and less ultra-violet energy for forming secondary products, Figure 4. The nitrogen dioxide pattern is less distinct with less variation from month to month. Mean concentrations are higher in winter months when the rate of photolysis is lower, Figure 5. The highest monthly mean concentrations of oxidants occur during the period from late spring to early fall when the rate of photochemical reactions is highest, Figure 6.

For a long time it was believed that high oxidant concentrations regularly occurred only in urban areas. Recent studies of oxidants in rural areas have shown surprisingly high concentrations. In studies of ozone at selected sites in New York State, high ozone values occurred simultaneously in rural and urban areas. Rural ozone levels did not tend to decrease to near zero at night. It is possible that high rural ozone levels are due to the transport of ozone and ozone precursors from urban areas, to reactions of naturally occurring precursors, or to transport of ozone from the stratosphere to the troposphere.[7,8] In another study of high levels of ozone in rural areas it was suggested that ozone clouds as much as 50 or 60 miles long could form downwind from electric power plants.[9] Monitoring at CAMP stations for 1964 - 1973 has shown that a large downward trend in oxidant concentration has been

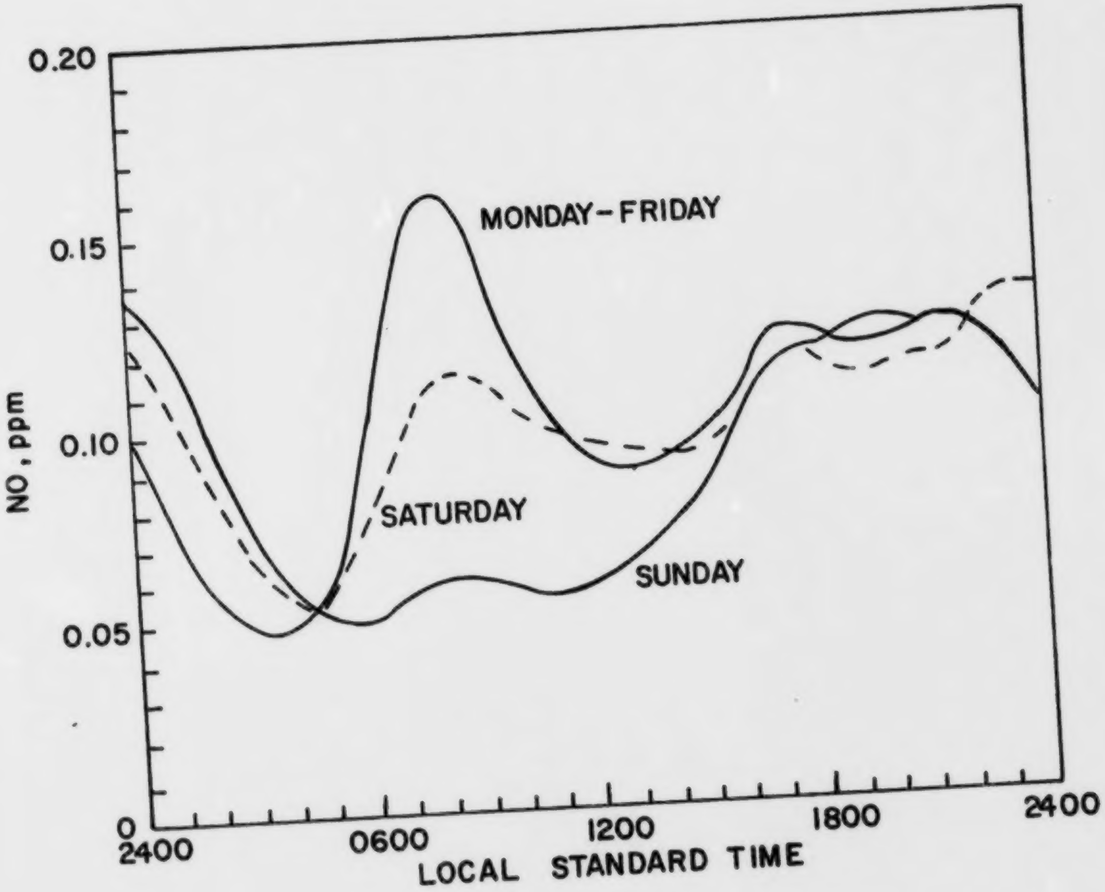


Figure 2. Weekday and weekend 1-hour average NO levels in Chicago, 1962 through 1964[2]

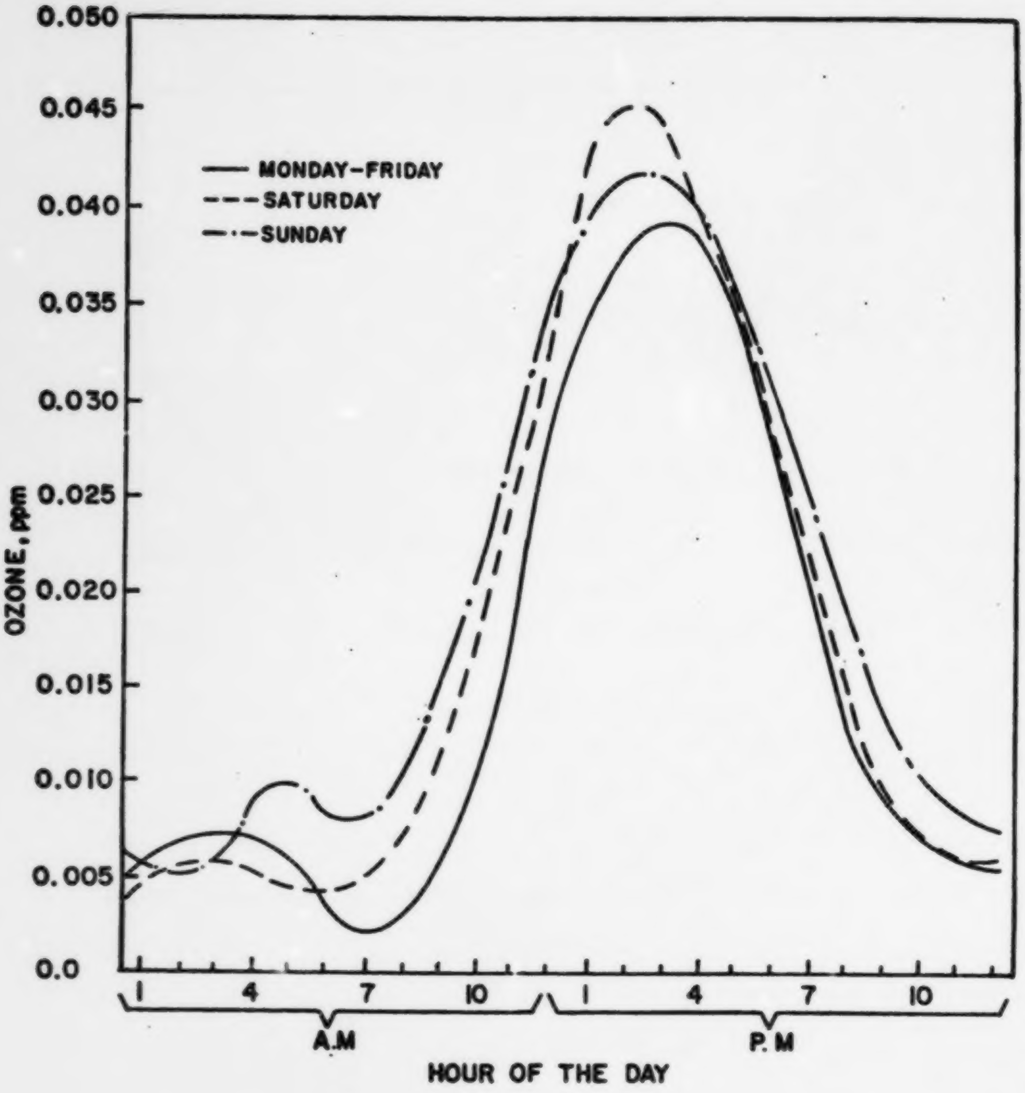


Figure 3. Diurnal variation of O_3 at Welfare Island for Monday through Friday, Saturday and Sunday[5]

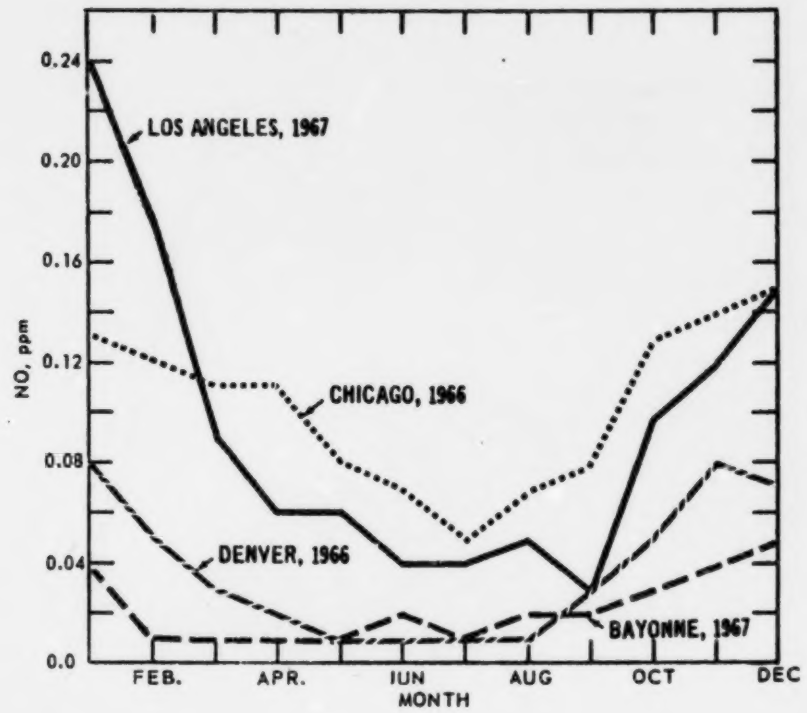


Figure 4. Monthly mean NO concentrations at four urban sites[2]

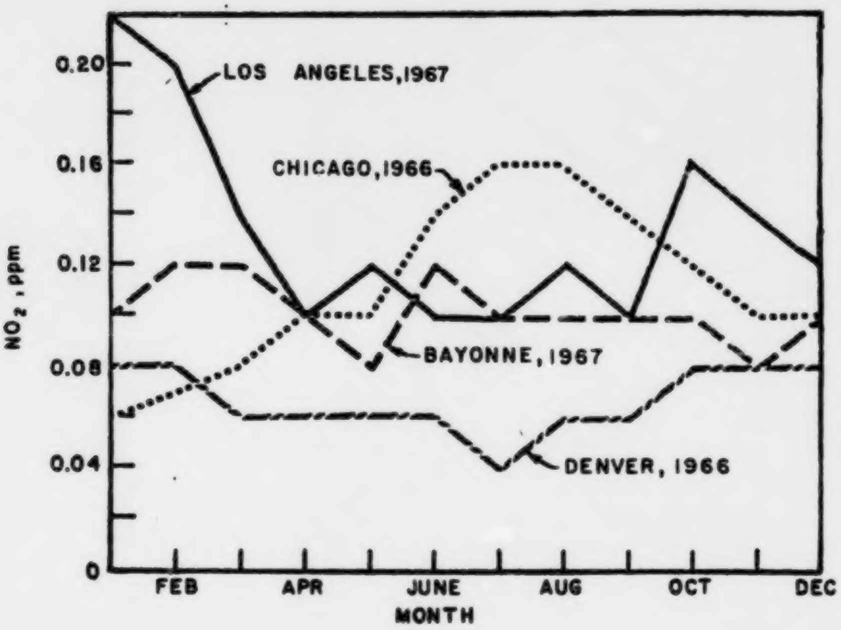


Figure 5. Monthly mean NO_2 concentrations at four urban sites[2]

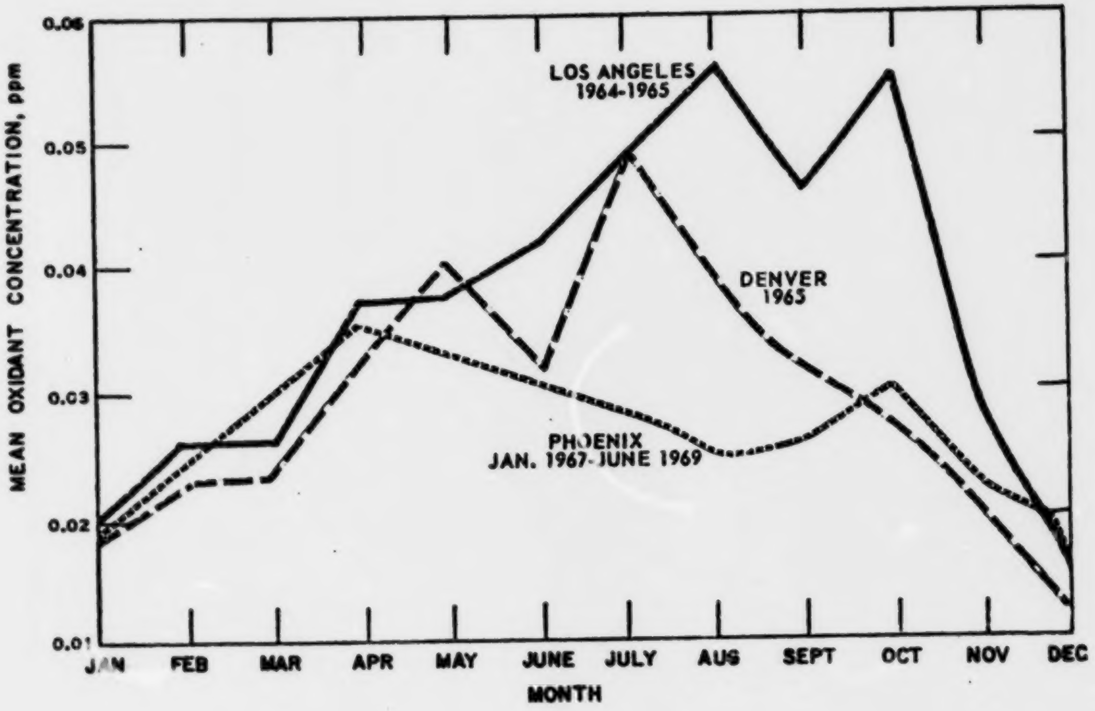


Figure 6. Monthly variation of mean hourly oxidant concentrations for three selected cities[1]

occurring but the factors responsible for this trend in the central business districts may not be causing similar reductions at suburban or downwind sites.[4]

A study of the vertical distribution of oxidants showed that concentrations may increase by factors of from 2 to 10 at higher altitudes within the mixing layer.[10] Below 10,000 feet, this appears to be the result of urban air pollutant emissions and subsequent photochemical reactions. This suggests that ozone buildup in advected air masses is primarily the result of a continuous photochemical aging of the air mass. The smaller ground level ozone measurements probably result from physical quenching on surfaces and/or chemical quenching.

It appears, then, that problems with high oxidant concentrations are not confined to urban areas - natural sources and long-range transport, both horizontally and vertically, are factors which seem to be making oxidants a regionwide, and probably nationwide, problem.

QUANTITATIVE RELATIONSHIPS OF OXIDANTS AND PRECURSORS

The appearance of oxidants in the urban atmosphere is dependent upon chemical reactions. These chemical reactions in turn are dependent on variables such as sunlight, wind and temperature as well as atmospheric dilution and dispersion. Because of the numerous variables involved, the relationship between precursor emissions and atmospheric oxidant concentrations is indirect and difficult to quantify. Nonlinearity characterizes the photochemical system.[1]

A study was performed to attempt to define the relationship of hydrocarbons to oxidants in ambient atmospheres of several cities.[11] The only assumption made was that there exists a relationship between early morning average hydrocarbon concentrations and subsequent maximum hourly average oxidant concentrations. In order to define the hydrocarbons which were likely to become involved in oxidant forming reactions, the average concentrations of nonmethane hydrocarbons from

6 to 9 a.m. were determined. A measure of nonmethane hydrocarbons is a better measure of the reactive hydrocarbons than total hydrocarbons is, even though not all nonmethane hydrocarbons are considered reactive. It was found that at any given hydrocarbons level, there exists a limit on the amount of oxidant which can be generated, Figures 7 and 8. The atmospheric conditions that lead to maximum oxidant potential occur on about 1 percent of all days so the maximum oxidant concentration for a given hydrocarbons concentration is reached only infrequently. The average 6 to 9 a.m. concentration of 0.3 ppm C nonmethane hydrocarbons can produce a maximum hourly average oxidant concentration of up to 0.1 ppm. Greater nonmethane hydrocarbons concentrations may also produce the same oxidant concentration but under extreme atmospheric conditions, a minimum concentration of 0.3 ppm C is sufficient.

Appendix J of 40 CFR 51 is a graph of the reduction in hydrocarbon emissions required to achieve the national standard for photochemical oxidants concentration, Figure 9. The graph is based on the results of the study of the relationship between total hydrocarbons and resultant oxidant levels discussed above. Appendix J does not use the nonmethane hydrocarbons relationship with oxidant which might, perhaps, be more accurate. Also, it assumes that there is no hydrocarbon or oxidant background - considering the recent studies which were discussed, this appears to be an invalid assumption.

Oxidant concentration has also been studied as a function of both 6 to 9 a.m. hydrocarbons and oxides of nitrogen concentrations.[12] Figure 10 shows the pollutant relationships for Los Angeles. It suggests that there is an optimum hydrocarbon/oxides of nitrogen ratio with respect to maximum attainable oxidant concentration. A reduction in hydrocarbons with no change in oxides of nitrogen results in a reduction in oxidant. But a reduction only in oxides of nitrogen may sometimes result in an increase in oxidant.

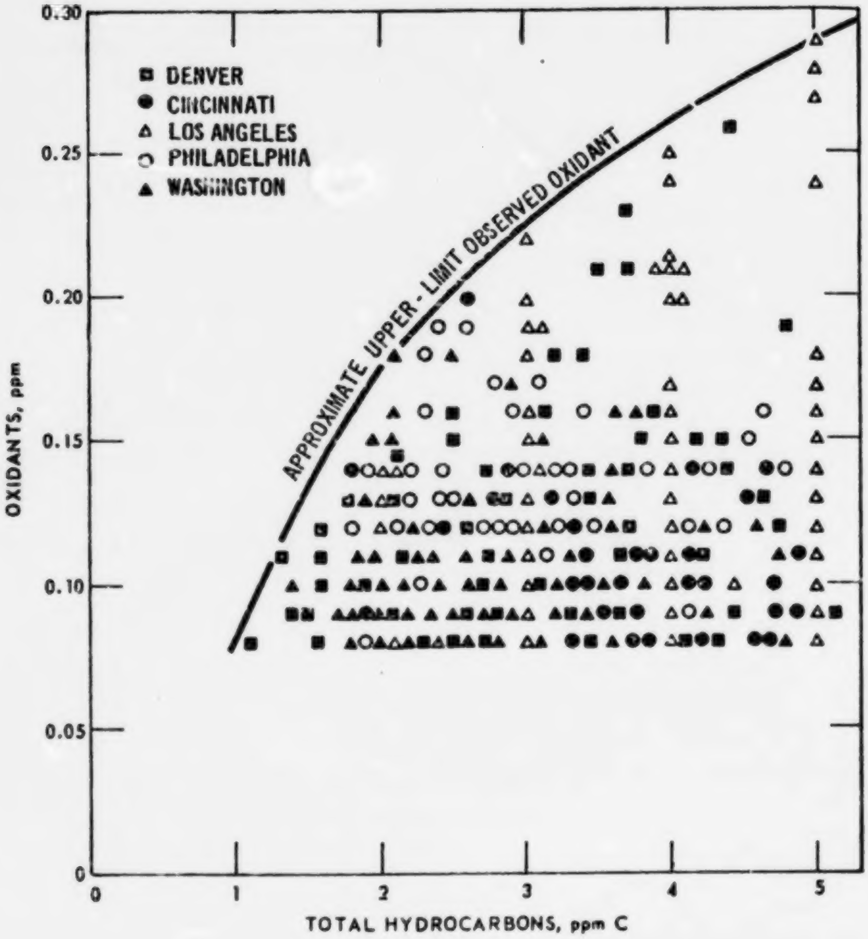


Figure 7. Maximum daily 1-hour average oxidant concentrations as a function of 6- to 9-a.m. averages of total hydrocarbon concentrations at CAMP stations, June through September, 1966 through 1968 and in Los Angeles, May through October 1967[10]

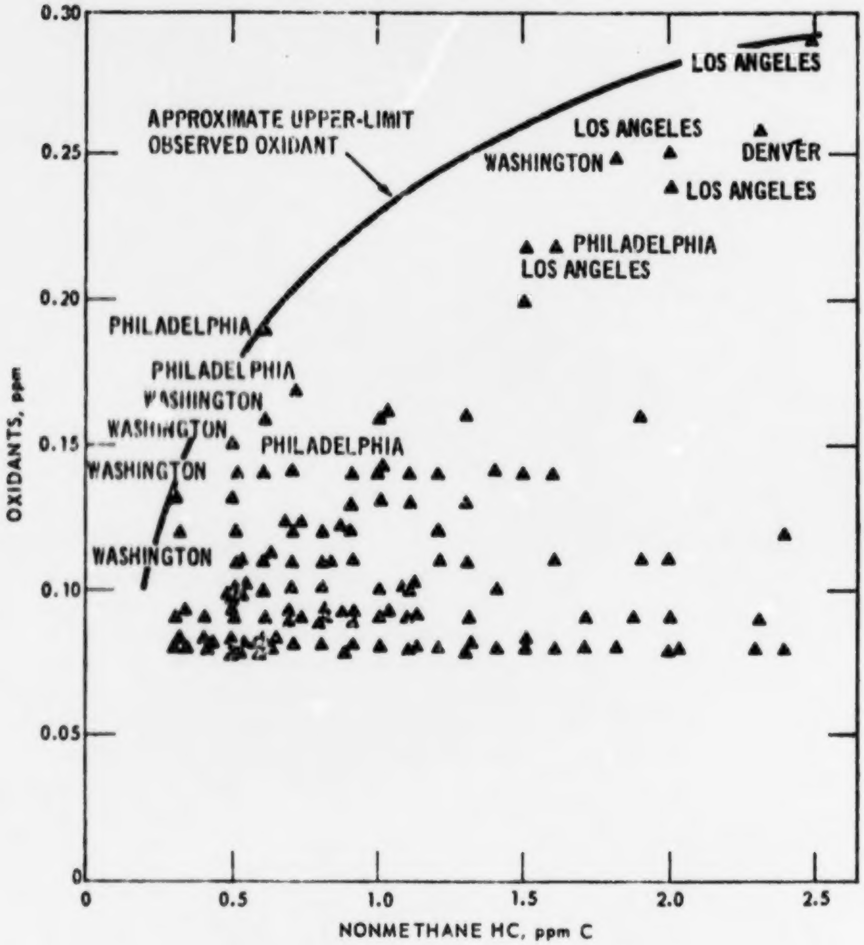


Figure 8. Maximum daily 1-hour average oxidants as a function of 6- to 9-a.m. averages of nonmethane hydrocarbons at CAMP stations, June through September, 1966 through 1968, Los Angeles, May through October 1967[10]

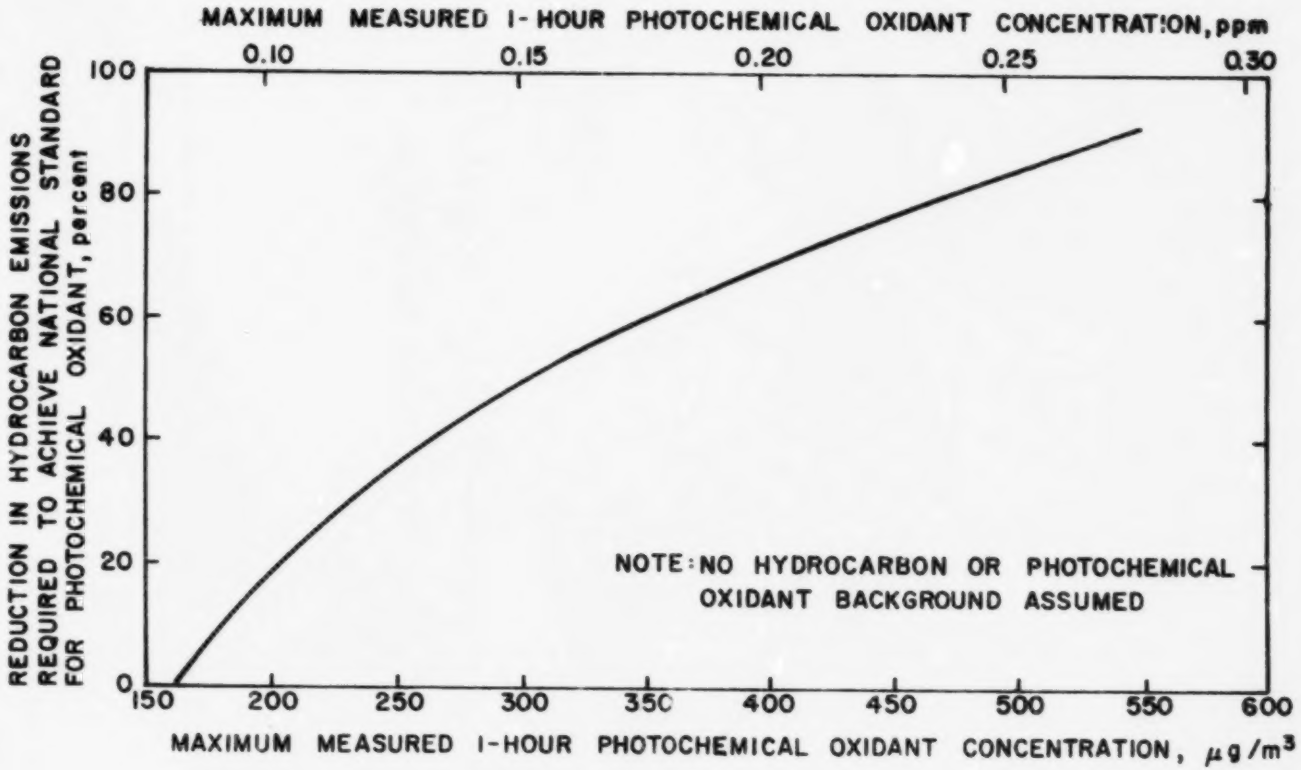


Figure 9. Required hydrocarbon emission control as a function of photochemical oxidant concentration (40 CFR 51)

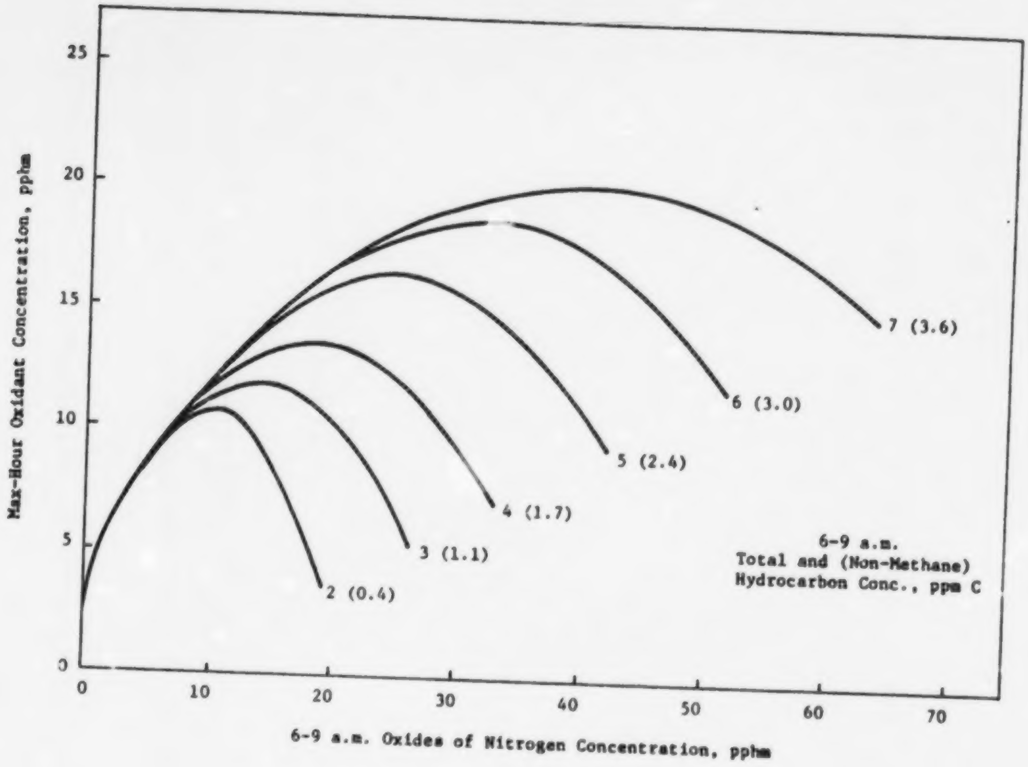


Figure 10. Pollutant relationships at Los Angeles, data period: July to September 1969 to 1972[11]

These graphs are among the simpler models attempting to define the relationship of oxidants with their precursors - hydrocarbons and nitrogen oxides. Complex air pollution models have been developed with varying degrees of reliability and include proportional rollback, rollback along a precursor curve, and dispersion modeling. These are discussed in a companion document, "Photochemical Oxidant Modeling Techniques Applicable to Highway System Evaluation," GCA/Technology Division, June 1975.

REFERENCES

1. Air Quality Criteria for Photochemical Oxidants. PHS, EHS, NAPCA, Publication Number AP-63, March 1970.
2. Air Quality Criteria for Nitrogen Oxides. PHS, EHS, NAPCA, Publication Number AP-34, January 1971.
3. Elkus and Wilson. Air Basin Pollution Response Function: The Weekend Effect. Submitted to Science.
4. Altschuller. Evaluation of Oxidant Results at CAMP sites in the United States. JAPCA, 25 (1): 19, January 1975.
5. Bell Laboratories. Statistical Analysis and Phenomenological Interpretation of the Atmosphere in the New York - New Jersey Metropolitan Region.
6. Cleveland, et al. Sunday and Workday Variations in Photochemical Air Polutants in New Jersey and New York. Science, 186: 1037, DC 1974.
7. Stasiuk and Coffey. Rural and Urban Ozone Relationships in New York State. JAPCA, 24 (6): 565, June 1974.
8. Coffey and Stasiuk. Evidence of Atmospheric Transport of Ozone into Urban Areas. ES and T, 9 (1): 59, January 1975.
9. Power Plant Gases Source of Puzzling Rural Ozone Clouds. Science News 106:260.
10. Gloria, et al. Airborne Survey of Major on Basins in California. JAPCA, 24 (7): 645, July 1974.
11. Schuck, et al. Relationship of Hydrocarbons to Oxidants in Ambient Atmospheres. JAPCA, 20 (5): 297, May 1970.
12. Paskind and Kinosian. Hydrocarbon, Oxides of Nitrogen and Oxidant Pollutant Relationships in the Atmosphere Over California Cities. Presented at APCA.

SECTION IV

OXIDANT MODELING ACTIVITIES

In our initial review of techniques for the prediction of NO_x and oxidant levels, four models were investigated, three of which can be classified as complex computer models requiring a wide range of input parameters. One of the models studied represented a rather simplified approach to the calculation of pollutant levels. A brief description of each of these air quality models is given below. It is beyond the scope of this report to give a detailed exposition of the internal workings of each of these models, particularly the more complex ones. References should be consulted if more information concerning a particular technical point is desired. Details of the model operations will be treated in some depth, however, if a thorough understanding of a given point is needed for successful application of the model by a potential user.

In addition to these four models, an assessment was made of the Appendix J technique for estimating oxidant/hydrocarbon reduction relationships based on data from Denver. This section begins with a discussion of the Appendix J results. Following this, the four models are discussed. The remainder of this section describes the application of two of these models in the Denver area.

APPENDIX J RESULTS

To assess how well the Appendix J nonlinear rollback method would work for Denver, it would have been desirous to construct an upper-limit curve for Denver, based on maximum daily 1-hour average oxidant concentrations as a function of 6:00 a.m. to 9:00 a.m. averages of total hydrocarbon concentrations, and then to convert this to an Appendix J type curve showing the reduction in hydrocarbon emissions required to meet the oxidant standard as a function of the maximum measured 1-hour oxidant concentration. Unfortunately, there were not sufficient data to define an unambiguous upper-limit curve.

As an alternative, sets of two or more consecutive days were chosen for which the oxidant standard was exceeded on the first day but not violated on the last day. These sets are listed in Table 1, along with the 6:00 a.m. to 9:00 a.m. average hydrocarbon concentrations, the percent reduction in hydrocarbon concentration on successive days (a surrogate for emissions also assumed in Appendix J), and the approximate reduction in hydrocarbons necessary to meet the oxidant standard as predicted by Appendix J. In most instances, oxidant levels fall below the standard with less percent reduction in hydrocarbons than predicted by Appendix J. This is not of great consequence, however, since these oxidant-hydrocarbon pairs fall below the upper-limit curve on which Appendix J is based. Of greater interest is sets 2 and 4. During the first 2 days in each of these sets, plotted oxidant-hydrocarbon pairs would lie above the Appendix J basis upper-limit curve. This would imply that a lower concentration of hydrocarbons would be associated with a given concentration of oxidant than is given by the upper-limit curve on which Appendix J is based. If the upper-limit curve were to include these hydrocarbon-oxidant pairs, a smaller percent reduction in hydrocarbons to meet the oxidant standard would be reflected by a shift downward in the Appendix J curve.

GENERAL MODEL DESCRIPTIONS AND INPUT REQUIREMENTS

Urban Air Shed Photochemical Simulation Model,[1,2] (SAI Model)

Of all the models studied, this model, which was developed by Systems Applications Inc. (SAI) for the EPA Meteorology Laboratory, provides the

Table 1. DATA SETS FOR APPENDIX J DISCUSSION

Set	O_x[a]	HC[b]	% HC[c] reduction	Appendix J[d]
1	412	4079		
	78	3724	8.7	70
2	549	2061		
	549	1507	26.9	90
	78	1352	10.3	90
3	196	1795		
	59	2305	-28.4	20
4	529	1374		
	529	2106	-53.3	85
	59	1795	14.8	85
5	196	1552		
	78	1729	-11.4	20
6	196	2327		
	39	2261	2.8	20
7	176	2017		
	98	1419	29.7	10
8	216	2372		
	59	1795	24.3	22
9	176	2372		
	98	1574	33.6	10
10	274	1685		
	59	1751	-3.9	40
11	196	1818		
	127	1773	2.5	20
12	196	2172		
	143	1286	40.8	20
13	225	1862		
	294	1662	10.7	30
	225	1485	10.7	50
	176	1951	-31.4	30
	88	1906	2.3	10

[a] $\mu g/m^3$ measured as ozone by chemiluminescence.

[b] $\mu g/m^3$ total hydrocarbons.

[c] Percent reduction from previous day's concentration.

[d] Approximate percent reduction required to meet the standard.

most detailed treatment of the physical and chemical processes important in the formation of photochemical smog. Concentrations of reactive species are determined by means of a finite difference scheme for an array of grid cells. Meteorological inputs to the program consist of wind speed and direction for a number of stations in the area. These values are then interpolated to give a flow vector for each ground level grid. Each grid cell is also assigned an hourly mixing depth which depends upon the terrain elevation and the measured mixing depth at one or more meteorological stations. The input of initial concentrations and hourly meteorological variables for specified measurement locations is handled by means of data preparation programs. These programs also determine correlations among corresponding input parameters at various stations, so that measured values may be extended over the entire grid system.

The SAI model also employs a rather sophisticated emission inventory routine for mobile and stationary sources. In addition to standard inputs such as vehicle-miles traveled (VMT) for different road types, the emissions submodel requires such detailed information as airport emissions for different aircraft types, mole fraction of NO in auto NO_x emissions, and correction factors for each pollutant species to account for the non-uniform distribution of vehicle starts.

The most important advantage of the SAI model over the other two complex computer models we investigated is its ability to predict concentrations for all grid squares at a particular time. This high degree of spatial resolution is obtained at the expense of long running times (1 hour simulation = 10 hours real time). Another disadvantage in applying the model to any given city is the fact that some aspects of the program are quite specific to Los Angeles. In particular, for the correlation of wind speeds, wind directions, and mixing depths, the Los Angeles basin is subdivided within the program itself into a number of topographically similar regions. Another drawback to the application of the SAI model from the viewpoint of a potential user is the inability to specify different values of horizontal and vertical diffusion coefficients without making modifications to the program itself. This situation seems curious in light of the significant role played by these variables in the determination of ozone and NO_x concentrations and the extensive amount of computer time required for the simulation of these diffusion effects.

In spite of the fact that the SAI model is an excellent research tool, it was felt that the long running times and extensive data requirements would make it difficult for a 3-C planning agency to use the model for analysis of different transportation strategies without a considerable investment in time and manpower.

Reactive Environmental Simulation Model (REM)[3,4]

The second computer model which we examined was developed for EPA Meteorology Laboratory by Pacific Environmental Services, Inc. Although the model utilizes a complex chemical reaction module, its approach toward the problem of atmospheric transport and dispersion is much simpler than for the SAI model. Rather than trying to predict hourly pollutant concentrations for every grid point, the REM employs a coordinate system which moves along a particular wind trajectory. Unlike the SAI model, the REM does not provide for either vertical or lateral transport by turbulent diffusion. The reaction volume may be considered to be a cylinder of unit cross sectional area bounded on top by the mixing height and on the bottom by the ground surface. The pollutants entering the bottom of the cylinder are assumed to be instantaneously uniformly mixed throughout the cylinder volume, which assumes the role of a reaction chamber. The wind speed and direction data are handed in much the same manner as in the SAI model but the emissions inventory is much less detailed. For example, the emission factor used for both freeways and surface streets does not appear to be corrected for the different speeds on the two different road types.

One of the most attractive features of this trajectory approach is the short computing time (1 hour simulation time = 150 hours real time for the IBM 370/155). The main drawback in the REM is the neglect of turbulent diffusion in the vertical direction. With this in mind we turned our attention to another trajectory approach which does consider this process.

Diffusion/Kinetics Code[5,6] (DIFKIN)

As in the case of the REM, DIFKIN calculates the trajectory of an air parcel across an emission grid network and determines time dependent concentrations of reactive pollutants. The equation for turbulent diffusion in the vertical direction is solved to obtain concentrations and fluxes for as many as five mesh points from the ground surface to the top of the mixing layer. DIFKIN requires that reaction rates and stoichiometric coefficients be read in as data for each model run, thereby facilitating any updates which may be required for the chemical system. The model also allows for trajectories to be run backward in time, a feature which is necessary to determine trajectory starting points so that the air parcel under study will pass over a measurement station.

Since DIFKIN utilizes its own emission calculation routines it was not necessary to input emission rates externally, although the program does provide for that option. Provision is also made for the input of stationary source emissions of both NO_x and HC.

Due to the reasonable running time (≈2 minutes IBM 370/158 time for each trajectory) and the relative ease of program modification compared to the SAI model, we selected the DIFKIN model as a tool for the study of NO_x and O_3 impact due to planned projects under the 3-C process. This decision was not meant to imply that the SAI model was technically deficient, but that its current level of complexity would make its routine use by a 3-C planning agency quite difficult. This problem might be alleviated in the future with the development of better data preparation programs. While the DIFKIN model is less specific to Los Angeles than the SAI model, a minor amount of reprogramming was necessary before the model was ready to run for the Denver area. This activity will be discussed more fully in a later section.

A Simple Dispersion Model for the Analysis of Chemically Reactive Pollutants[7]

For the past several years F. A. Gifford and S. R. Hanna of the Atmospheric Turbulence and Diffusion Laboratory (ADTL) at Oak Ridge, Tennessee have been active in the development and validation of simple methods for estimating pollutant concentrations in urban areas. Much of their effort had been restricted to the analysis of chemically inert pollutants, but they have recently generalized their model to treat pollutants undergoing photochemical reactions.

The Gifford-Hanna model is basically a "box model" in which average pollutant concentrations within the box are taken to be proportional to the ratio of the average area source strength to the wind speed. The proportionality constant is set equal to the average width of the region divided by the average depth of the pollutant cloud over the area. This depth is allowed to vary as a function of atmospheric stability and may be calculated by an integration of the Gaussian plume formula over the extent of the area source.

For purposes of chemical kinetics calculations the pollutant concentrations are assumed to be uniform within the volume defined by the area of the region and the depth of the pollutant cloud. By nondimensionalizing the concentrations which appear in the equations governing chemical reactions, it is possible to gain some insight into the importance of a particular reaction upon the concentration of a particular species. For instance, if the steady state nondimensionalized concentration of a particular substance is close to unity, it is possible to neglect chemical transformation for the associated meteorological conditions and emission rates.

The reaction scheme utilized in this model was originally proposed by Friendlander and Seinfeld[8] and may be written in terms of the following four equations.

$$\frac{\partial}{\partial t}\left[NO_2\right] = \left[NO_2\right]\left[RH\right]\left(\alpha\left[NO\right] - \lambda\left[NO_2\right]\right) \tag{1}$$

$$\frac{\partial}{\partial t}\left[NO\right] = -\alpha\left[NO_2\right]\left[NO\right]\left[RH\right] \tag{2}$$

$$\frac{\partial}{\partial t}\left[RH\right] = -\left[NO_2\right]\left[RH\right]\left(\theta + \frac{\mu}{\left[NO\right]}\right) \tag{3}$$

$$\left[O_3\right] = \beta\frac{\left[NO_2\right]}{\left[NO\right]} \tag{4}$$

where $\alpha = \frac{1}{600}\ \mathrm{ppm}^{-2}\ \mathrm{sec}^{-1}$

$\mu = \frac{1}{2.4 \times 10^5}\ \mathrm{sec}^{-1}$

$\theta = \frac{1}{3 \times 10^4}\ \mathrm{ppm}^{-1}\ \mathrm{sec}^{-1}$

$\lambda = \frac{1}{3 \times 10^3}\ \mathrm{ppm}^{-2}\ \mathrm{sec}^{-1}$

$\beta = 0.02$ ppm

$\left[NO\right]$ = nitric oxide concentration (ppm)

$\left[NO_2\right]$ = nitrogen dioxide concentration (ppm)

$\left[RH\right]$ = reactive hydrocarbon concentration (ppm)

$\left[O_3\right]$ = ozone concentration (ppm)

The concentrations in equations (1) through (4) are indicated in brackets. No functional dependence with solar radiation intensity is specified for these reaction rates. Nondimensionalized concentrations $\left[C\right]^*$ and times t^* may be found from the following transformations:

$$\left[C^*\right] = \frac{\left[C\right] UZ}{Q\ \Delta x} \qquad (5)$$

$$t^* = \frac{t\ U}{\Delta x} \qquad (6)$$

where $\Delta x = A\ Z$

U = wind speed (m/sec)

Q = emission density ($\text{cm}^3\ \text{m}^{-2}\ \text{s}^{-1}$)

A and Z in turn depend upon the stability of the atmosphere for the particular day in question. The variation of these two parameters with stability is shown in Table 2. Equations (1) through (3) can then be written in terms of nondimensionalized concentrations and times.

$$\frac{\partial}{\partial t^*} \ln\left[NO\right]^* = \frac{1}{\left[NO\right]^*} - 1 - \left[NO_2\right]^*\left[RH\right]^*\ C1 \qquad (7)$$

$$\frac{\partial}{\partial t^*} \ln\left[NO_2\right]^* = \frac{1}{\left[NO_2\right]^*} - 1 + \left[NO\right]^*\left[RH\right]^*\ C2 - \left[NO_2\right]^*\left[RH\right]^*\ C3 \qquad (8)$$

$$\frac{\partial}{\partial t^*} \ln\left[RH\right]^* = \frac{1}{\left[RH\right]^*} - 1 - \left[NO_2\right]^*\ C4 - \left(\left[NO_2\right]^* / \left[NO\right]^*\right)\ C5 \qquad (9)$$

where $C1 = \alpha Q_{NO_2}\ Q_{RH}\ \dfrac{\Delta x^3}{U^3\ Z^2}$ (a) (10)

$C2 = \alpha Q_{NO}\ Q_{RH}\ \dfrac{\Delta x^3}{U^3\ Z^2}$ (b)

$C3 = \lambda Q_{NO_2}\ Q_{RH}\ \dfrac{\Delta x^3}{U^3\ Z^2}$ (c)

$$C4 = \Theta \, Q_{NO_2} \frac{\Delta x^2}{U^2 Z} \qquad (d)$$

$$C5 = \mu (Q_{NO_2}/Q_{NO}) \frac{\Delta x}{U} \qquad (e)$$

Q_i = emission rate of substance i ($cm^3\ m^{-2}\ s^{-1}$)

Table 2. VARIATION OF DIFFUSION PARAMETERS WITH STABILITY CONDITION

Parameter	Stability condition		
	Unstable	Neutral	Stable
A	50	200	600
Z	2000m	150m	40m

Two approaches are possible for utilizing equations (7) through (9) in the prediction of ozone and NO_x levels. The first option is to assume that the process has reached a steady state so that the time derivative on the left side of the equations can be set to zero. The equations may then be solved algebraically for the nondimensionalized concentrations. These may then be redimensionalized and compared with measured values. Since the steady state approximation may not strictly be applied due to the time variation of emission density and solar radiation intensity, it is open to some question which hour should be chosen for the comparison of measured and "steady state" values. In his Los Angeles validation study Hanna picked the noon hour for a comparison.

The second way in which the model may be applied is actually to solve the chemical kinetics equation numerically by use of a Runge-Kutta technique to obtain values for nondimensionalized concentrations as a function of time. If an hour such as 6:00 a.m. is chosen as the time when all nondimensionalized concentrations are equal to 1, then the time variation of the wind speed, emission rate, and nondimensionalized concentrations may be used to project actual concentrations from their 6:00 a.m. values.

The assumptions made concerning the emissions estimates are no less severe than those dealing with chemical reaction rates. The ratio of NO_2 to NO emissions is set equal to the $\left[NO_2\right]/\left[NO\right]$ concentration ratio at 6:00 a.m. The following relationships are also assumed to hold between RH and NO_x emissions:

$$Q_{NO} = 0.3\ Q_{RH} \qquad (a) \qquad\qquad (11)$$

$$Q_{NO_2} = 0.2\ Q_{RH} \qquad (b)$$

In spite of the rather drastic approximations made in the development of this model, it was felt that it should be applied along with the more detailed complex approaches due to the extensive data requirements and computing time required for their application.

SELECTION OF TEST MODELS

In the previous section we briefly touched upon our reasons for the selection of the DIFKIN model over the SAI and REM models in our test of the application of complex photochemical models to the 3-C planning process. The following four selection criteria were employed during the screening process.

- Technical accuracy
- Program modifications required for application to a new location
- Input requirements
- Computer time

The REM model was ruled out early in the study due to the assumption inherent in the calculation that the pollutants within a moving column of air are always uniformly mixed. Another technical difficulty with the model is failure to include the effect of speed in vehicular emissions. These problems outweigh any advantages due to simplified model operation and the relatively small amount of computer time required for photochemical simulation.

While the SAI model is the technically superior of the three complex models, it falls short in the other three categories. To run the SAI model for an area different from the Los Angeles basin would require extensive modifications in the data preparation programs to include the topographic effects of the new area. Also, the quality of emissions and meteorological data required for the program would require a data gathering effort out of proportion with that required for other 3-C planning activities unless much of this information had been generated from previous studies. And finally, the treatment of both horizontal and vertical diffusion effects for a large number of grid cells requires excessive amounts of computer time.

Although the SAI and DIFKIN models require similar input data bases, the number of necessary program modifications and the amount of computer time required for program operation are less prohibitive for the latter model. These two factors were considered more important than the lack of a capability to predict hourly concentrations for each grid cell.

A common failing with all three complex models is the lack of any clear indication as to which variables the model is most sensitive. It is not obvious to the potential user how his time may be most profitably spent in the collection of data. For example, the user is uncertain whether more resources should be devoted to a more accurate specification of different highway speeds or a better determination of the diffusion profile. While several paragraphs of a users manual may be devoted to a discussion of a plotting routine, there is often little guidance concerning more important inputs such as initial reactive hydrocarbon concentrations. In general we feel that before any of these more complex models can be more widely applied, a more user-oriented operations manual will be required.

EVALUATION OF THE DIFKIN MODEL

We shall now describe the steps used to evaluate DIFKIN as a tool for the analysis of NO_x and oxidant impact of actions taken as a part of the 3-C planning process. It is important to remember that this evaluation is based upon our actual experience in applying the model to the Denver area, so that the associated difficulties and necessary program modifications would be similiar to those encountered in a modeling effort carried out by a planning agency. In this connection, the first part of our discussion will be devoted primarily to the data preparation and operational aspects of DIFKIN, as opposed to the details of the theoretical formulation. Since, in the final analysis, the model must be judged on the basis of its predictive capability, we shall report on an actual model evaluation effort using hourly air quality and meteorological data for a particular day.

Model Application to Denver

One fact to bear in mind when applying a photochemical model to a given urban area is that most models were designed and validated based upon measurements taken in the Los Angeles area. This is understandable in light of the extensive monitoring network, the well studied local inversion phenomenon, and the absence of significant emission sources outside the Los Angeles basin. There is no real guarantee that the DIFKIN model, once validated using the Los Angeles data base, will accurately account for O_3 and NO_x levels in other major urban centers where the presence of higher levels of SO_2 and suspended particulates may alter the reaction scheme. An even more important consideration is the selection of initial pollutant concentrations for the air parcel used in DIFKIN.

Aside from any potential technical difficulties which may arise in the application of a photochemical simulation model to a new area, there remains the task of data preparation and even program modification necessary for successful operation of the code. The reprogramming effort is a particularly bothersome task since it involves the removal or replacement of actual program statements and block data entries specific to the Los Angeles basin validation site. We shall now treat in somewhat greater detail the modifications required so that the DIFKIN model could be run for Denver.

Required Program Modifications

The DIFKIN program and Los Angeles test data set were obtained from Dr. Kenneth Demerjian of the EPA Meteorology Laboratory, Research Triangle Park, North Carolina. The code, which was originally written by General Research Corporation (GRC) to run on an IBM 370 computer, had been translated by EPA personnel to operate on a UNIVAC 1108 system. The program modifications required so that DIFKIN could again be run on an IBM 370 included the following:

- The appropriate commands had to be inserted in the dummy DIFKIN subroutine SECOND to enable it to call IBM system routines capable of obtaining the internal machine time for the purpose of timing the DIFKIN computations.
- The UNIVAC machine language subroutine MCHAR, used for moving a string of individual characters from one storage location to another, had to be replaced by an equivalent IBM machine language subroutine.
- The backspace commands contained in SETPLT, the printer plot subroutine, were removed in order to minimize the number of disk actuations used in the running of the program. This may not be necessary when using other facilities where disk actuations are cost-effective.
- The control cards which govern the execution of the program had to be written to coordinate peripheral devices and the unit numbers representing them in DIFKIN and the IBM computer facilities. Fourteen disk files had to be properly defined for DIFKIN use.

The following DIFKIN program modifications were required for the incorporation of a new data base:

- The appropriate wind station names and coordinates, compass point azimuths, and distance criteria were inserted in SETIN, a DIFKIN subroutine called upon to initialize the aforementioned variables.
- Subroutine BARIER, a routine which checks whether or not two given points are on the same side of a straight line barrier, had to be altered to remove the effect of Los Angeles topographical features such as the San Gabriel mountains, Santa Monica mountains, and Palos Verdes hills. Interpolation of wind speed and direction measurements for trajectory calculations is not permitted between those stations located on opposite sides of a barrier. No barrier was utilized for Denver since the mountains west of the city do not pass between wind measurement stations.
- BLOCK DATA programs ONE through FIVE were changed so that mobile and stationary source emission parameters for Denver could be entered.

Application Results

Input Data Base - The input requirements of the DIFKIN program may be clearly separated into emissions, meteorological, and photochemical. Of these three categories the emissions input constitutes the largest volume of data necessary for the operation of the code. Most of it is actually contained within the program itself in the form of data statements within Block Data Subprograms listed in Appendix A.

The first block data subprogram contains data statements for the following arrays:

1. FFWY - This two dimensional array consists of average daily freeway VMT (k mi) for each of 625 grid cells superimposed upon the Denver meteorpolitan area.
2. FSRF - This array is identical to FFWY except that it contains surface street VMT data.

3. FXNO2, FXHCR - These two arrays are filled with 625 values for distributed NO_2 and reactive hydrocarbon emissions, respectively.

4. FPPNO2, FORNO2, FORHCR - These three arrays contain coordinates and emission strengths for power plant NO_2 emissions, oil refinery NO_2 emissions, and oil refinery reactive hydrocarbon emissions. Space is provided for up to 30 power plants and oil refineries. This input option was not utilized in DIFKIN run for Denver (i.e., zeros were entered for the coordinate values and emission strengths). All NO_2 and reactive hydrocarbon emissions were assigned to the arrays FXNO2 and FXHCR. The model treats power plant and oil refinery emissions no differently from other emissions except that separate adjustment factors are provided.

As mentioned previously, the block data format required for the emissions input makes even slight changes in the data base quite cumbersome. For example, the two dimensional array FSRF is equivalenced to four one dimensional arrays due to a restriction to the number of lines in the data statement.

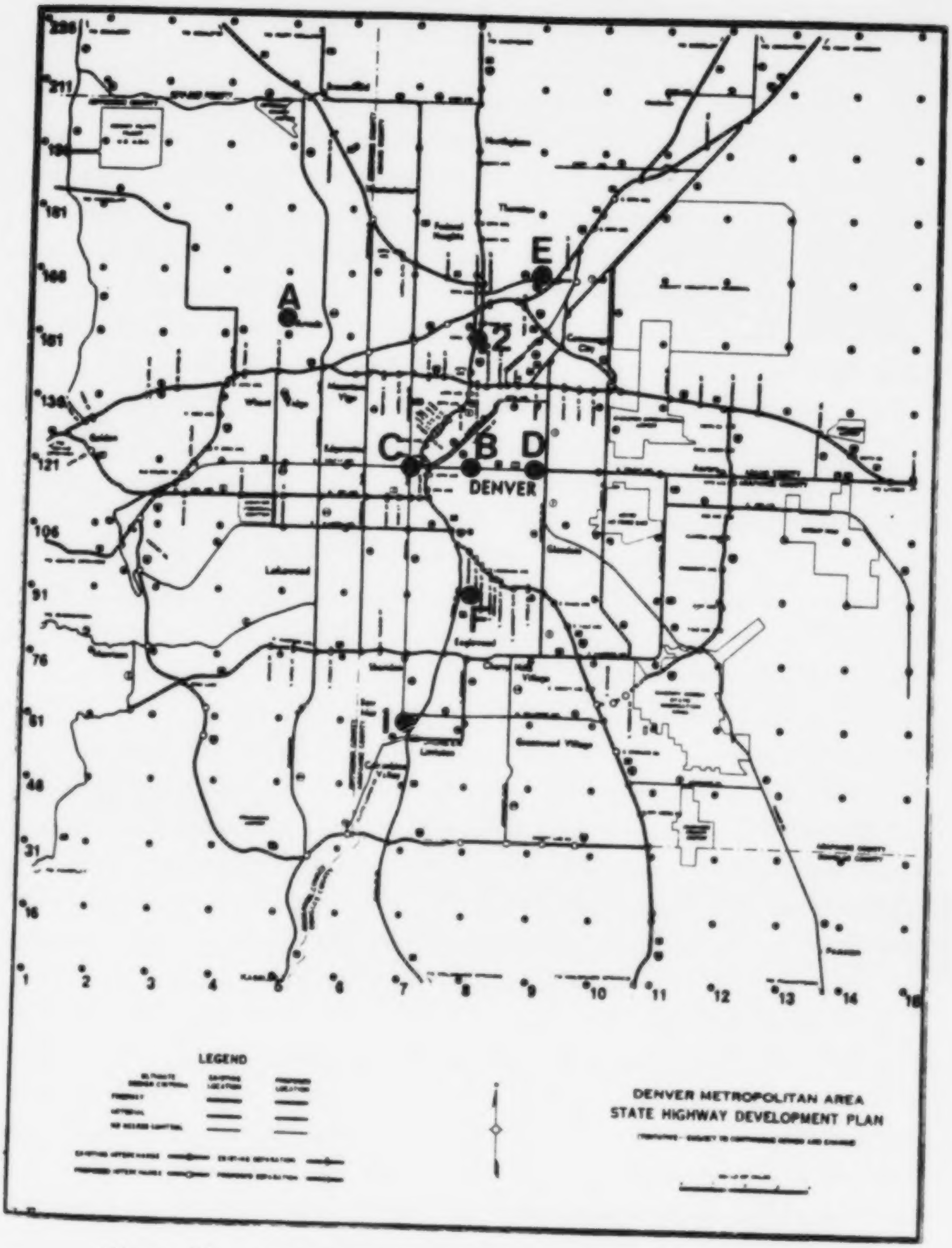
The freeway and surface street VMT data for Denver were obtained from the Colorado Division of Highways for the base year of 1972 and projected travel for the year 2000. Projected values for 1975 were found by simple interpolation. The original breakdown by road type was according to the following classifications:

Road classification	Average speed (mi/hr)
Freeway	40
Expressway	34
Primary arterial	26
Minor arterial	23
Collector	21
Centroid connector	20
Ramps	20
Major arterial	23

Both freeways and expressways were assigned to the DIFKIN freeway category and the remaining links were treated as surface streets. VMT data for each link were allocated to an appropriate 2 mi x 2 mi grid square by means of a program developed by the Colorado Division of Highways. The grid used in this procedure (see Figure 11) was a system of 16 rows and 15 columns previously developed as a coordinate system for the APRAC-1a[9] carbon monoxide simulation program. Listings of VMT data for freeways and surface streets based upon this grid system are given in Tables 3(a) and (b). This grid was modified by adding four rows on the top, five rows on the bottom, and five columns on each side so that it would conform to the dimensions required by the DIFKIN program. Emissions for these added grid cells were set equal to zero.

Stationary source emissions of NO_2 and reactive hydrocarbons were obtained for the Denver area through the EPA National Emissions Data System (NEDS) from a point source listing. The emission rates of NO_2 and reactive hydrocarbons in kg/hr, assigned to the appropriate grid squares are displayed in Table 4. Unfortunately there is no distinction made in NEDS between reactive and nonreactive hydrocarbons emissions or the fraction of NO and NO_2 in the oxides of nitrogen emission estimate. The values reported in Table 4 are total hydrocarbon and NO_x emissions. DIFKIN actually assumes that all NO_x emissions are really NO even if they are reported as NO_2, since the factor 30/46 (the NO to NO_2 molecular weight) is applied to all NO_x emissions both mobile and stationary.

The next two block data programs contain the arrays FSLOW6, FSLOW7, FSLOW8, FSLOW9, FFAST6, FFAST7, FFAST8, and FFAST9, which represent the peak average traffic speeds in the slow and fast direction for each hour between 6:00 a.m. and 9:00 a.m. for all 625 grid squares. These data were based primarily upon field observations in the Denver area by GCA and its subcontractor Wilbur Smith and Associates.


226
211
181
166
151
136
121
106
91
76
61
46
31
16
A
E
2
C
B
D
DENVER
F
1
1
2
3
4
5
6
7
8
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10
11
12
13
14
15
LEGEND
DENVER METROPOLITAN AREA
STATE HIGHWAY DEVELOPMENT PLAN

Figure 11. Map of the Denver Metropolitan Area showing air monitoring stations (lettered) and wind stations (numbered)

Table 3(a). DAILY FREEWAY VMT (k mi) FOR DENVER (1973)

FW

0	0	0	45	2	0	0	43	0	0	0	28	10	5	0
0	0	0	0	81	0	0	48	0	0	16	22	9	0	0
0	0	0	0	21	61	0	78	0	7	45	6	0	0	0
0	0	0	0	8	53	14	108	0	54	0	0	0	0	0
0	0	0	0	0	0	59	248	83	37	0	0	0	0	0
0	0	0	0	9	43	3	208	94	44	0	0	0	0	0
0	24	28	72	66	67	169	357	130	97	89	54	23	9	0
1	25	17	9	5	0	174	0	0	6	0	22	0	7	12
0	0	66	68	100	141	176	169	0	4	0	21	0	0	0
0	0	1	2	3	0	0	76	143	28	0	24	0	0	0
0	0	2	7	28	47	66	36	54	106	20	15	0	0	0
0	0	4	7	0	0	9	0	0	87	7	0	0	0	0
0	0	0	1	0	0	4	0	0	0	50	0	0	0	0
0	0	0	0	2	4	5	2	1	1	35	0	0	0	0
0	0	0	0	0	0	0	0	0	0	26	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 3(b). DAILY SURFACE STREET VMT (k mi) FOR DENVER (1973)

SS

0	0	0	8	20	0	2	0	1	0	1	2	6	0	0
6	3	4	5	33	26	18	32	10	2	4	2	5	0	0
7	2	7	6	4	12	29	103	15	9	7	6	0	1	0
6	2	8	2	3	34	61	102	39	13	6	0	0	1	0
0	7	7	6	30	92	133	106	38	61	7	3	0	1	0
0	5	13	30	113	147	100	82	51	42	14	2	3	1	0
0	22	15	37	102	227	269	202	210	134	22	51	10	2	0
2	38	40	66	171	252	256	633	400	262	206	117	29	10	3
0	10	7	42	109	205	236	438	299	146	99	64	14	0	0
0	0	2	23	84	165	174	313	262	144	63	10	2	0	1
0	0	3	6	23	77	80	278	128	87	54	15	1	0	1
0	0	0	5	27	18	153	139	64	28	23	4	3	0	0
0	0	0	0	20	23	50	78	57	27	20	10	16	0	0
0	0	0	0	10	31	25	15	14	4	1	0	8	2	0
0	0	0	0	24	4	9	0	0	0	0	0	0	6	0
0	0	0	0	8	0	3	0	0	0	0	0	0	0	0

Table 4. STATIONARY SOURCE EMISSIONS FOR NO$_x$ AND HC FOR THE DENVER METROPOLITAN AREA

```
NOX EMISSIONS IN KG/HOUR

   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   1.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   4.   0.   0.   0.   0.   0.   0.   3.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.  12.   0.   0.   0.   0.   0.   0.   0.   4.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   1. 369.  96.   0.   0.  25.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   1.   2.   0.   0.   3.  25.   4.   0.   4.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.  51.   2.   0.   0.   0.   3.   9.   0.   4.   0.   8.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   4.   0.   8.   0.   1. 154.   3.  25.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.  65.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0. 544.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   1.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   1.   0.   3.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.  11.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.

HC EMISSIONS IN KG/HOUR

   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   1.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.  66.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.  13.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.  21.  13. 249.   0.   0.  13.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.  58.   1.   0.   2.   2.  22. 113.  12.  25.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0. 133.   2.   0.   0.   0.   1.  77.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   8.   0.   1.   0.   0.  51.   3.   8.   0.   8.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0. 204.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.  10.   3.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   3.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   4.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   9.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
```

The peak traffic (slow/fast) volume ratio on freeways for each hour between 6:00 a.m. and 10:00 a.m. is given in the fourth block data program. The corresponding array names are FRAT6, FRAT7, FRAT8, and FRAT9. These data were obtained in the same manner as the data in the second and third block data programs.

The speed correction factors (B(I), C(I), I=1,3) for NO_x, HC, and CO mobile source emissions, were changed to correspond to the AP-42 correction factors. The new input values are shown in Appendix A.

The second emissions related variable which was changed from the Los Angeles value was VBAR, the off-peak average speed on freeways. The value of 44 mi/hr was estimated with the aid of a Colorado Division of Highways publication[10] which deals with a calibration study of the present highway network. Input parameters for the arrays YFR (fraction of vehicle starts which are cold starts) and CSF (correction factors to account for emissions following cold starts) were left with the values used in the Los Angeles study. These last two variables played no role in our DIFKIN runs for Denver since hot running and cold start emission factors were set equal to one another.[11] Average speeds for the surface streets are set equal to 19.6 mi/hr in the program to correspond to the 1972 Federal Driving Cycle.

The two remaining emission related arrays which must be specified within the program itself are TFWY (fraction of total daily freeway VMT for each hour) and TSRF (fraction of total daily surface street VMT for each hour). Data statements for TFWY and TSRF are located in the DIFKIN subroutine FLXDAT.

The remainder of the emission inputs and all of the meteorological and photochemical input variables are read into the DIFKIN code as "problem control inputs." A complete list of these variables is given in the DIFKIN users manual and many of the entries may be generated with little difficulty. Table 5 presents a list of selected problem control

Table 5. SUMMARY OF THE MOST IMPORTANT EXTERNAL INPUTS FOR DIFKIN

Input number	Variable name	Description	Source of input value for Denver
2	TRAJEX	Wind trajectory is input from cards (YES) or computed internally (NO)	User option.
3	EXFLUX	Fluxes are input from cards (YES) or computed internally (NO)	User option.
6	MODTE, NAM, NPT, PT	Date, station name, number of compass points, and 24 digital azimuth readings	Colorado Department of Health, Air Pollution Control Division.
9	IDT, XLCL	Date and local clock time at trajectory initial point	For a backward running trajectory, the time and date should correspond to the desired measurement time for the station in question. IDT and XLCL were chosen as August 13, 1973 and 1200 hours respectively to simulate the highest oxidant levels for the validation day.
12	TTOTAL	Time duration of trajectory, hours	For a backward running trajectory, the initial startup time will be TTOTAL hours before XLCL.
13	DTSEC	Time interval between wind calculations, hours	Has to be an integral multiple of measurement interval. For our calculation we chose an interval of 1 hour.
15	ITF	Trajectory is to be generated forward (+1) or backward (-1) in time	Trajectory was generated backward in time to insure that the air parcel would pass over the measurement station at noon.
16	IRF	Wind measurements weighted as I/R if (01) or $1/R^2$ if (02)	The I/R factor was used, as was done in the sample calculation.
17	NC	Number of nearby measurement stations desired for each wind vector interpolation	All three wind stations were used in the interpolation.
22	NEMF	Average driving cycle emission factors excluding cold start effects, grams/mile	The average emission factors for NOx, HC, and CO were determined with the computation methodology outlined in AP-42 along with the vehicle age distribution for Denver.
23	CEMF	Driving cycle emission factors with emissions from one cold start, grams/mile	The same emission factors were used as input 22 since a recent study.[11] Using DIFKIN concluded that ozone and nitrogen dioxide increases were "practically insignificant" when cold start emissions are included.
37	DELZ	Height of one cell of space mesh in meters	The height of 115 meters corresponded to the value used in the sample calculation.
38	SUNTIM	Time interval in minutes for updating NO_2 photodissociation rate constant, k	An interval of 10 minutes was chosen to correspond with the sample calculation.
53	NOSTAT	Number of vertical mesh points to be used	Following the sample calculation, 5 points were used.
56	PPHM	Initial concentration of each species at each mesh point in pphm	Since these concentrations would be associated with a parcel of air starting from a location far removed from the urban center, it was difficult to arrive at initial concentrations much less a concentration gradient in the vertical. Initial concentrations of NO_2, NO, HNO_2, and reactive HC were finally chosen as 1 pphm to approximate a parcel of clean air entering the city. Initial ozone concentrations were taken to be the initial ratio of k_1 to k_3. Initial CO concentrations were set equal to 2 ppm.
60	RATK1	Table of rate constants of NO_2 photodissociation reaction, k, in $minutes^{-1}$	The calculation of these input constants is based upon the technique outlined in Appendix C of the DIFKIN User's Guide.[6] The rates were increased by 10 percent to account for the higher elevation in Denver.
61	HTINV	Table of diffusion coefficients as functions of time and altitude, in meters squared per minute	Diffusion coefficients were determined by use of Figure 3.7 of the DIFKIN evaluation report which gives the diffusion coefficient profile for different stabilities.

inputs which are most significant for a potential user of the program along with an account for the manner in which each variable was assigned a value for the Denver test case. A full list of actual inputs used in the DIFKIN calculation is given in Appendix B.

The basic meteorological input to the program consists of hourly wind speed and direction measurements at a number of stations so that an air parcel trajectory can be determined. The locations of two of the three stations used in the Denver study are shown in Figure 11. The third station is located to the north of the smaller 15 × 16 grid. Hourly wind direction and speed values were obtained from the Colorado Department of Health, Air Pollution Control Division for the validation day of August 13, 1973.

Additional meteorological data for Denver Stapleton Airport were obtained from the National Climatic Center, Asheville, North Carolina for the year 1973. From these data we were able to extract information as to wind speed and cloud cover which could be used for atmospheric stability determinations, which could in turn be of some guidance in the specification of turbulent diffusivity profiles. The variation of diffusivity with height for different stability conditions is shown in Figure 12, taken from the document describing the DIFKIN model evaluation.[5]

The rate constants and stoichiometric coefficients for the DIFKIN chemical kinetics calculation were chosen to be those used in the sample calculation for Los Angeles with the exception of the hourly NO_2 photodissociation rate constant k_1. Hourly values for this reaction rate were developed for the validation day by use of a computer program similar to the one described in Appendix G of the DIFKIN users manual.

Concentration Measurements - Air quality data for 1973 were obtained from EPA Region VIII for the six monitoring sites in the Denver AQCR. The oxidant data (measured as ozone by chemiluminescence) were reviewed for days on which the 1-hour maximum concentrations exceeded the standard,

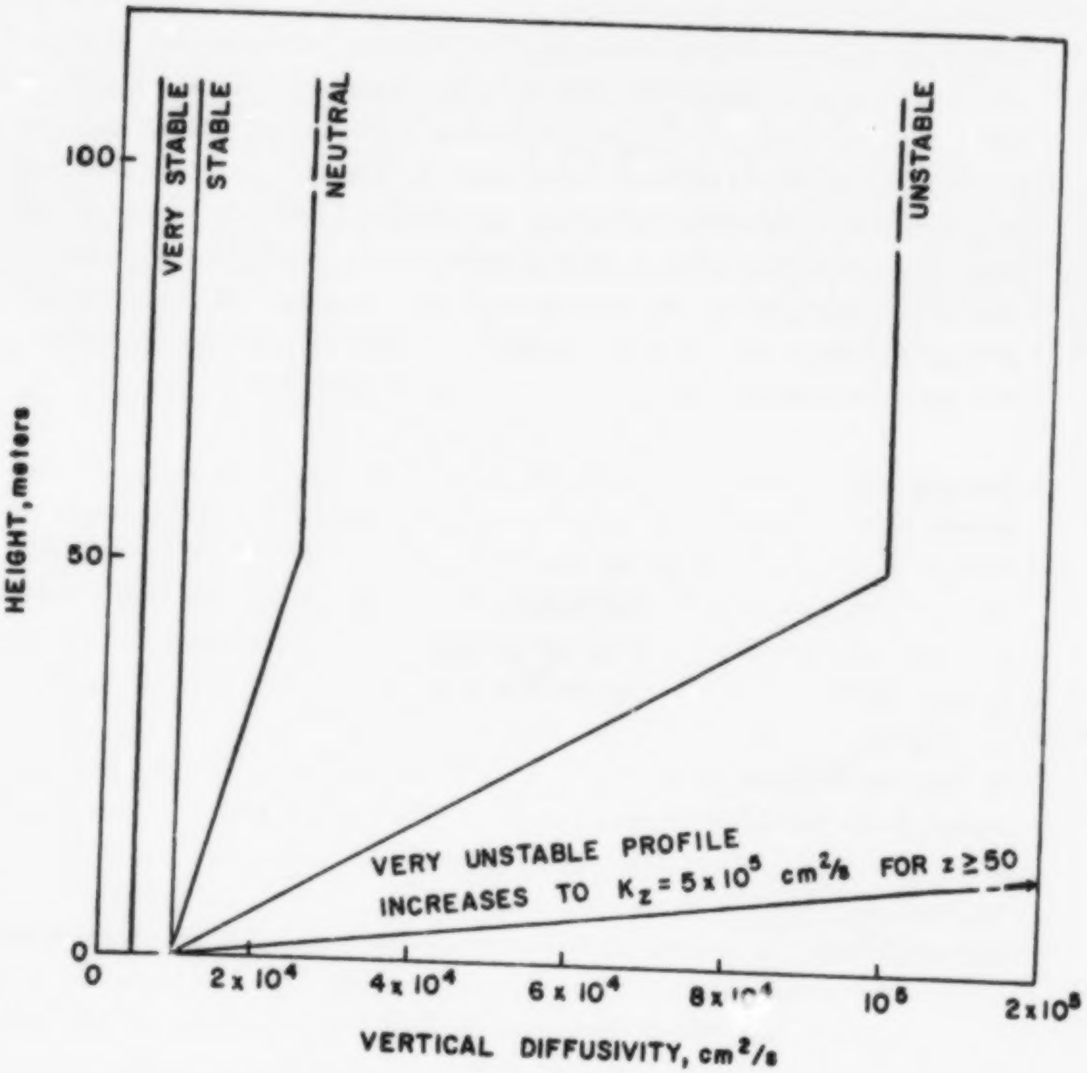

Figure 12. Variation of diffusivity with height for different stability conditions

since interest focused on how DIFKIN would perform on such days. Monday, August 13 was chosen for modeling since all five stations which were operating reported values exceeding the standard, allowing the largest number of spatial points at which to check DIFKIN calculated values. No other day had this many stations reporting a violation. Unfortunately, the station which was not operating this day was the only one measuring NO_2, and it ceased operation at the end of July. However, three of the remaining five stations commenced operation only in August, so August 13th was picked for its oxidant data at the expense of NO_2 data to compare with DIFKIN calculations. August 13, 1973 hourly concentrations for the Denver measurement stations are given in Table 6.

Test of Model Predictions - For the validation day, trajectory starting points were chosen so that the trajectory would end at a measurement station at 2 p.m. The actual procedure was to run the trajectories backward in time from a particular measurement location so that calculated and observed concentrations could be compared. In all cases the calculated starting point of the trajectories lay outside the city itself.

We then had to face the problem of specifying for the air parcel initial ground level air concentrations and concentration profiles of CO, RH, NO, NO_2, O_3, and HNO_2. Data from the measurement stations was no help in this task since they were far removed from the starting point of the trajectory. Another difficulty was the absence of reactive hydrocarbon (RH) measurements for the day in question. The decision was finally made to use the following background initial concentration values for the air parcel: $[CO] = 2$ ppm, $[RH] = 1$ pphm, $[NO] = 1$ pphm, $[NO_2] = 1$ pphm, and $[HNO_2] = 1$ pphm. The initial concentration of O_3 was set equal to the ratio k_1/k_2, where k_1 is the NO_2 photodissociation rate at the startup time of the trajectory and k_2 is the rate constant for the reaction: $NO + O_3 \rightarrow NO_2 + O_2$. All concentrations were assumed to be uniform with height above the ground. The concentrations and emission fluxes along five trajectories are displayed in Figures 13 through 17.

Table 6. SUMMARY OF AIR QUALITY AND METEOROLOGICAL DATA FOR THE VALIDATION DAY

Day	Hour	A			C			D			E			F			1	2	3
		HC[a]	CO[b]	Ox[a]	HC	CO	Ox	HC	CO	Ox	HC	CO	Ox	HC	CO	Ox	DIR/SPD[d]		
8/13/73	0000	-	0.3	49	2793	4.6	35	1995	4.0	20	1463	-	49	2128	2.3	-	21/03	18/04	V/02
	0100	-	0.3	69	2394	2.3	65	1795	3.4	35	1197	-	59	1862	2.3	-	21/03	29/07	30/03
	0200	-	0.3	69	2128	1.1	69	1463	2.3	49	1197	-	59	1463	1.1	-	21/03	29/12	36/05
	0300	-	0.3	69	1995	1.1	69	1596	2.3	55	1197	-	69	1463	0.3	-	21/02	31/15	03/09
	0400	-	0.3	69	1995	1.1	69	1529	2.3	49	1263	-	69	1463	0.3	-	03/07	31/13	36/11
	0500	-	0.3	45	2128	2.3	39	1729	3.4	35	1263	-	69	1596	1.1	-	33/05	31/07	36/07
	0600	-	2.3	29	2394	2.3	39	1862	4.0	29	1197	-	65	1596	3.4	-	36/06	31/03	03/04
	0700	-	1.1	59	1862	3.4	59	2261	5.7	59	1197	-	M	1463	3.4	49	33/03	34/01	05/05
	0800	-	1.1	84	1729	2.3	98	3059	5.7	176	1130	-	78	1729	4.6	65	27/02	31/03	09/05
	0900	-	3.4	M	1995	2.3	118	1995	5.7	118	1130	-	98	1729	5.7	127	27/02	31/04	12/05
	1000	-	3.4	167	2128	2.3	225	1862	6.9	M	1130	-	114	1862	5.7	255	03/03	V/03	15/07
	1100	-	3.4	274	2128	3.4	323	1795	6.9	235	1197	-	147	1729	5.7	314	06/04	06/05	15/05
	1200	-	3.4	382	2394	4.6	421	1729	5.7	304	1463	-	235	1463	4.6	216	21/03	V/04	18/07
	1300	-	4.6	470	2394	3.4	470	1729	5.7	319	1596	-	323	1463	4.6	314	24/03	V/05	16/07
	1400	-	4.6	500	2128	3.4	519	1663	4.6	261	1263	-	323	1330	4.6	294	27/03	V/03	18/05
	1500	-	4.6	490	1995	2.3	412	2527	8.0	172	1330	-	265	1330	4.6	225	36/04	34/04	18/05
	1600	-	3.4	392	2128	2.3	353	1995	6.9	147	1263	-	243	1330	4.6	255	03/05	36/04	03/05
	1700	-	3.4	372	2128	2.3	323	1995	4.6	162	1197	-	176	1596	5.7	323	36/05	34/07	36/05
	1800	-	3.4	235	2128	2.3	196	2128	5.2	98	1263	-	118	1729	5.7	245	36/06	34/07	33/06
	1900	-	3.4	143	2261	2.3	94	2394	8.0	65	1330	-	88	1729	4.6	88	36/08	31/09	04/08
	2000	-	3.4	153	2793	4.6	65	1862	6.9	49	1463	-	69	1995	5.7	76	33/04	02/06	09/03
	2100	-	3.4	104	2660	5.7	65	1596	4.0	35	2394	-	39	1596	3.4	65	18/03	V/02	18/03
	2200	-	2.3	108	2261	3.4	69	1596	4.0	39	2261	-	20	1995	3.4	49	21/04	18/07	21/04
	2300	-	3.4	86	1995	2.3	74	1596	3.4	39	2261	-	10	1596	2.3	69	21/04	16/08	24/06
	2400	-	2.3	88	1729	1.1	94	1330	2.3	78	1463	-	39	1330	2.3	84	24/04	18/08	21/07

[a] $\mu gms/m^3$ total carbon.

[b] $mgms/m^3$.

[c] degrees from north/10

[d] mph

Note: V = variable wind direction.

Air Quality Monitoring Stations:
A = W57th & Garrison Streets.
C = 2105 Broadway Street.
D = E. Colfax & Colorado Streets.
E = E78th & Steele Streets.
F = 2005 S. Huron Street.

Wind Stations:
1 = Centennial Wells.
2 = Denver Waste Water.
3 = Brighton.

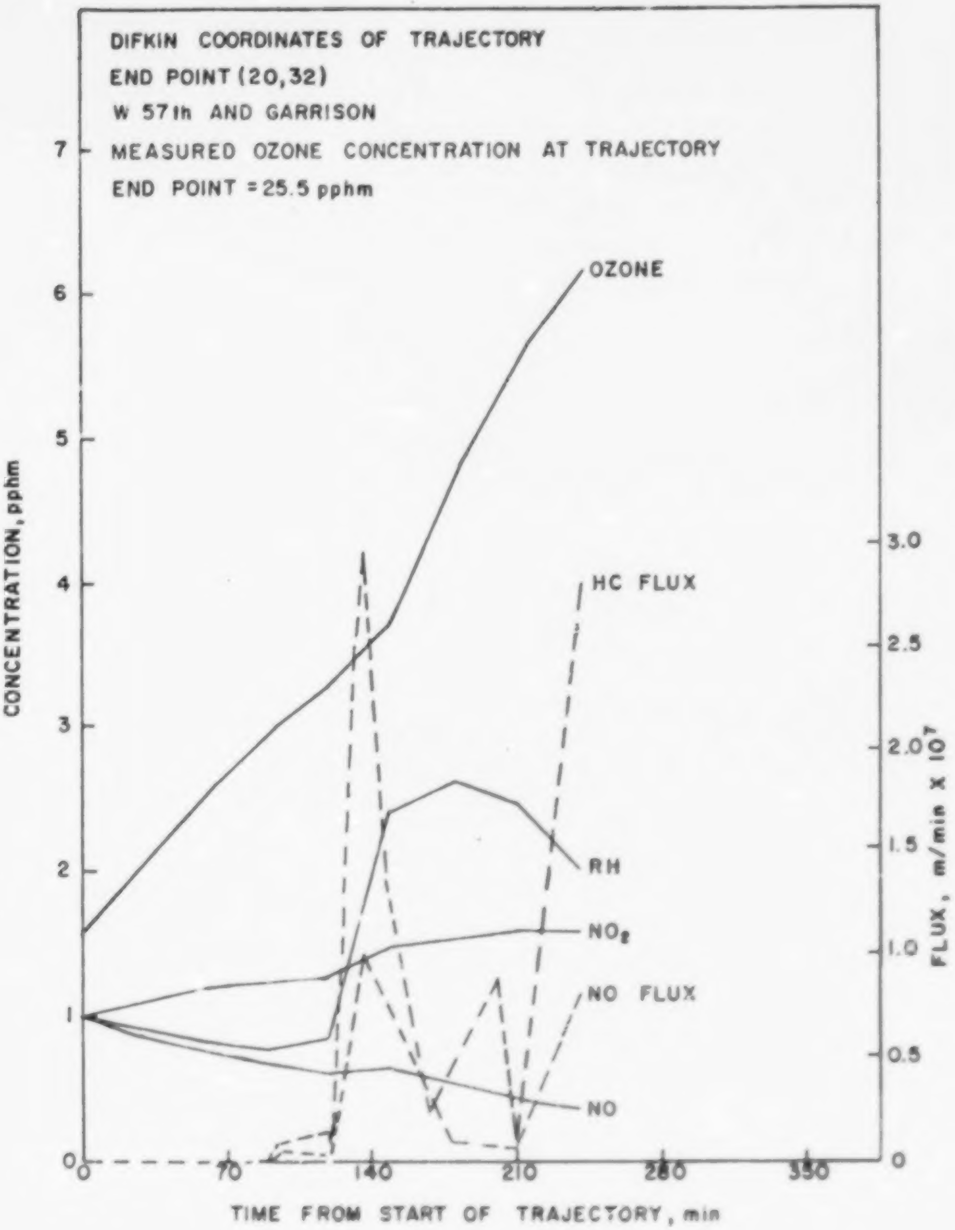

Figure 13. First DIFKIN evaluation run

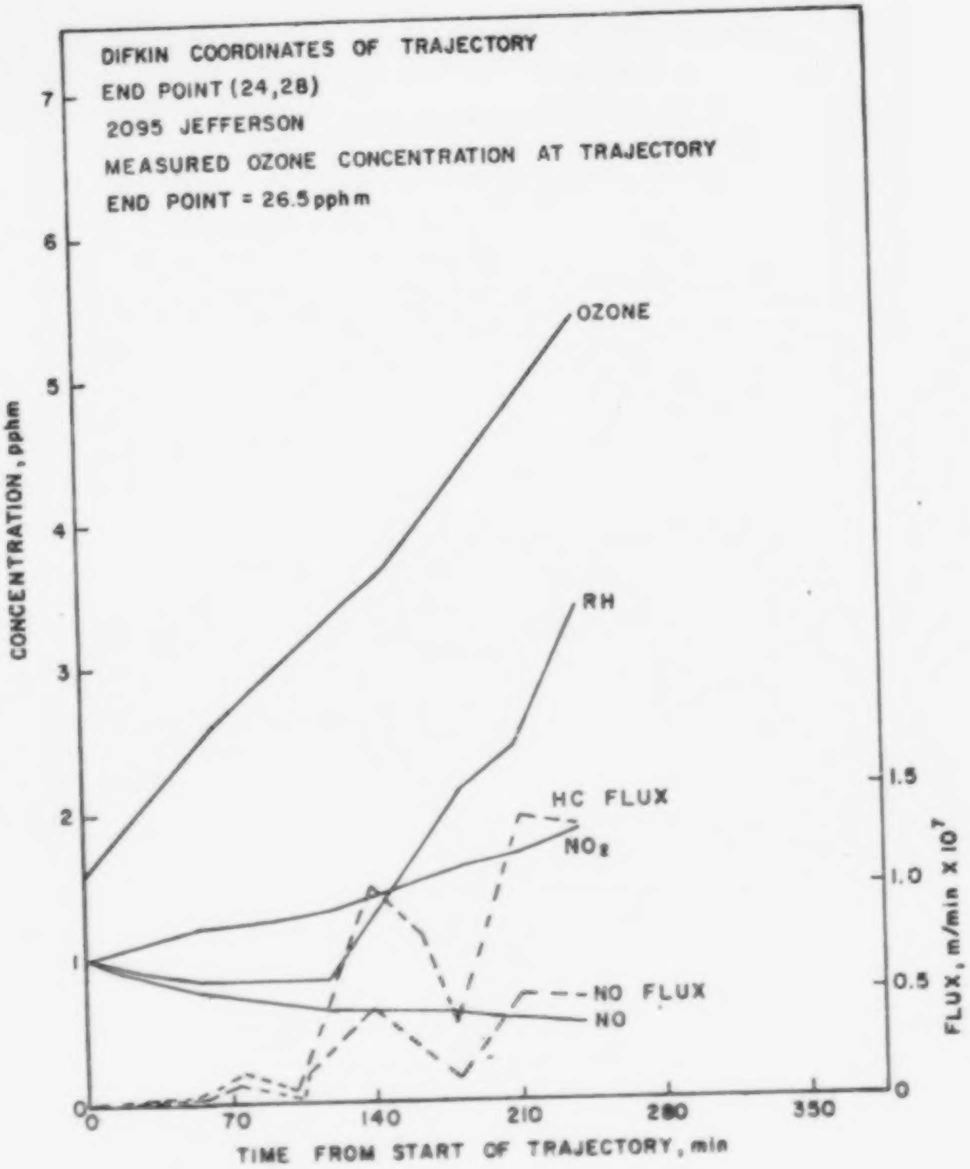

Figure 14. Second DIFKIN evaluation run

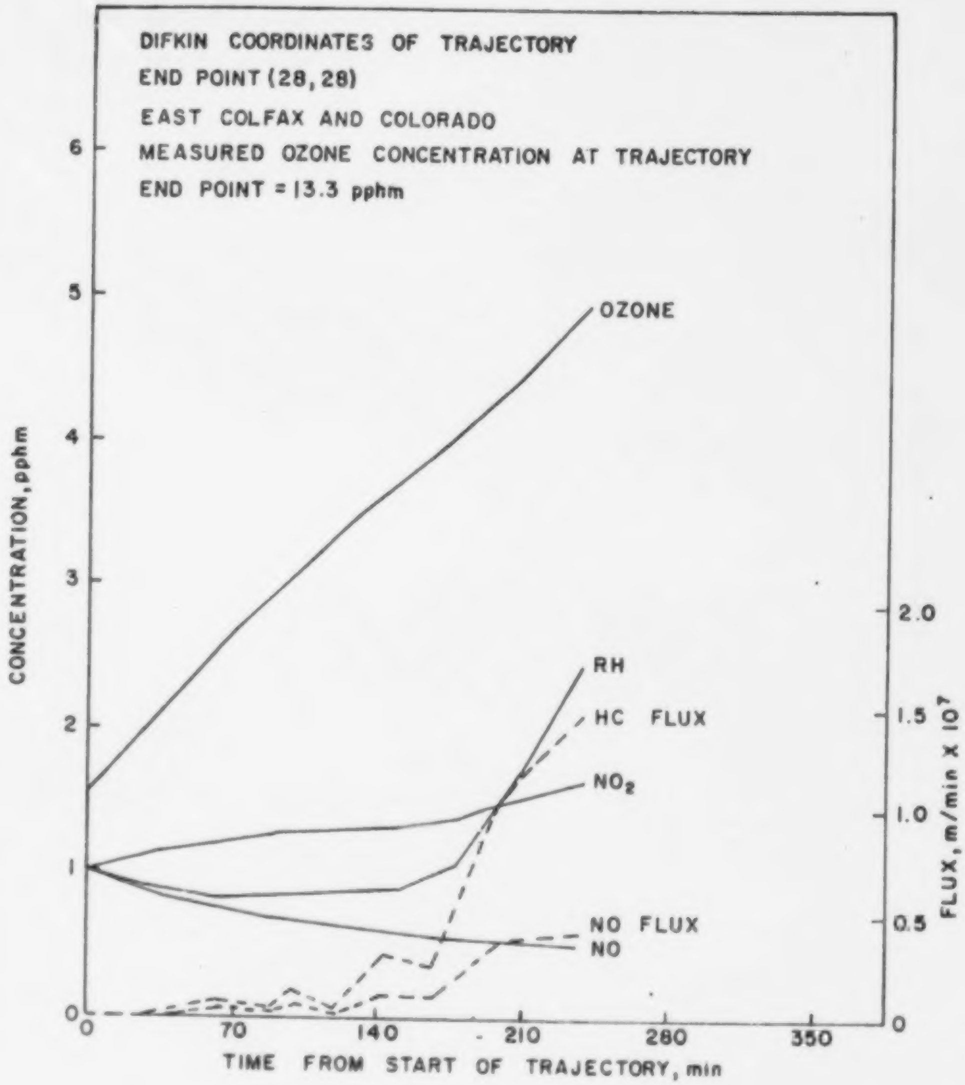

Figure 15. Third DIFKIN evaluation run

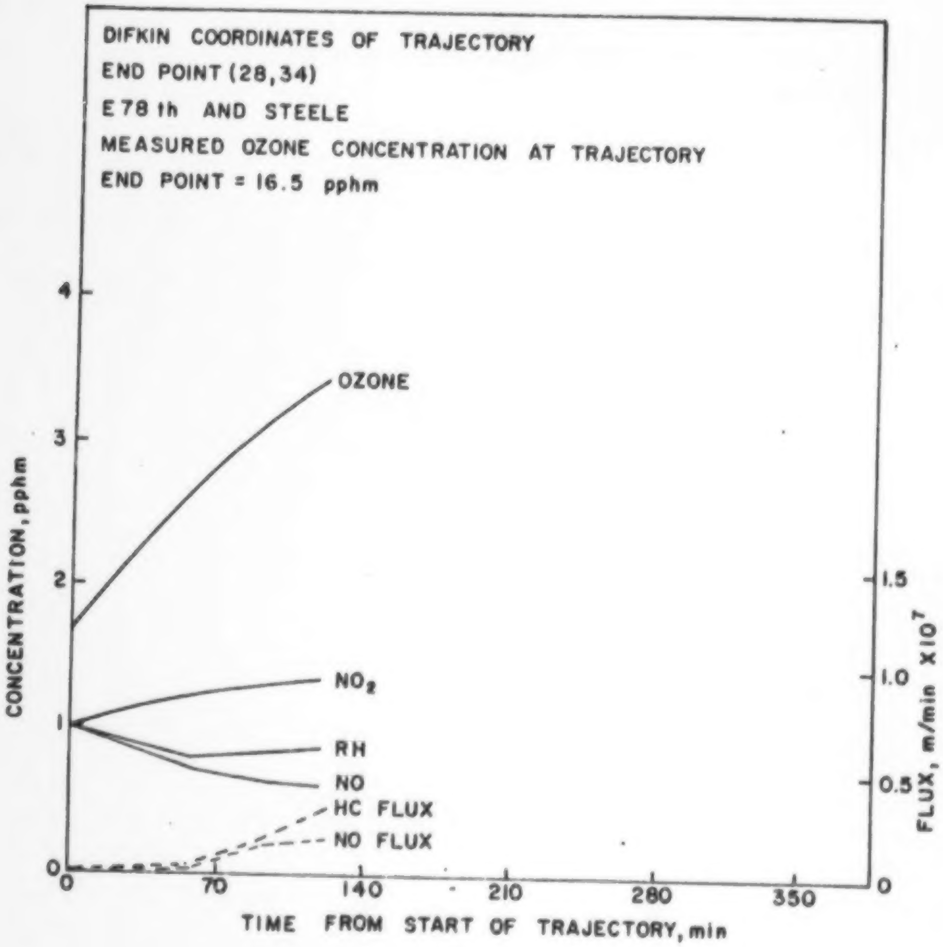

Figure 16. Fourth DIFKIN evaluation run

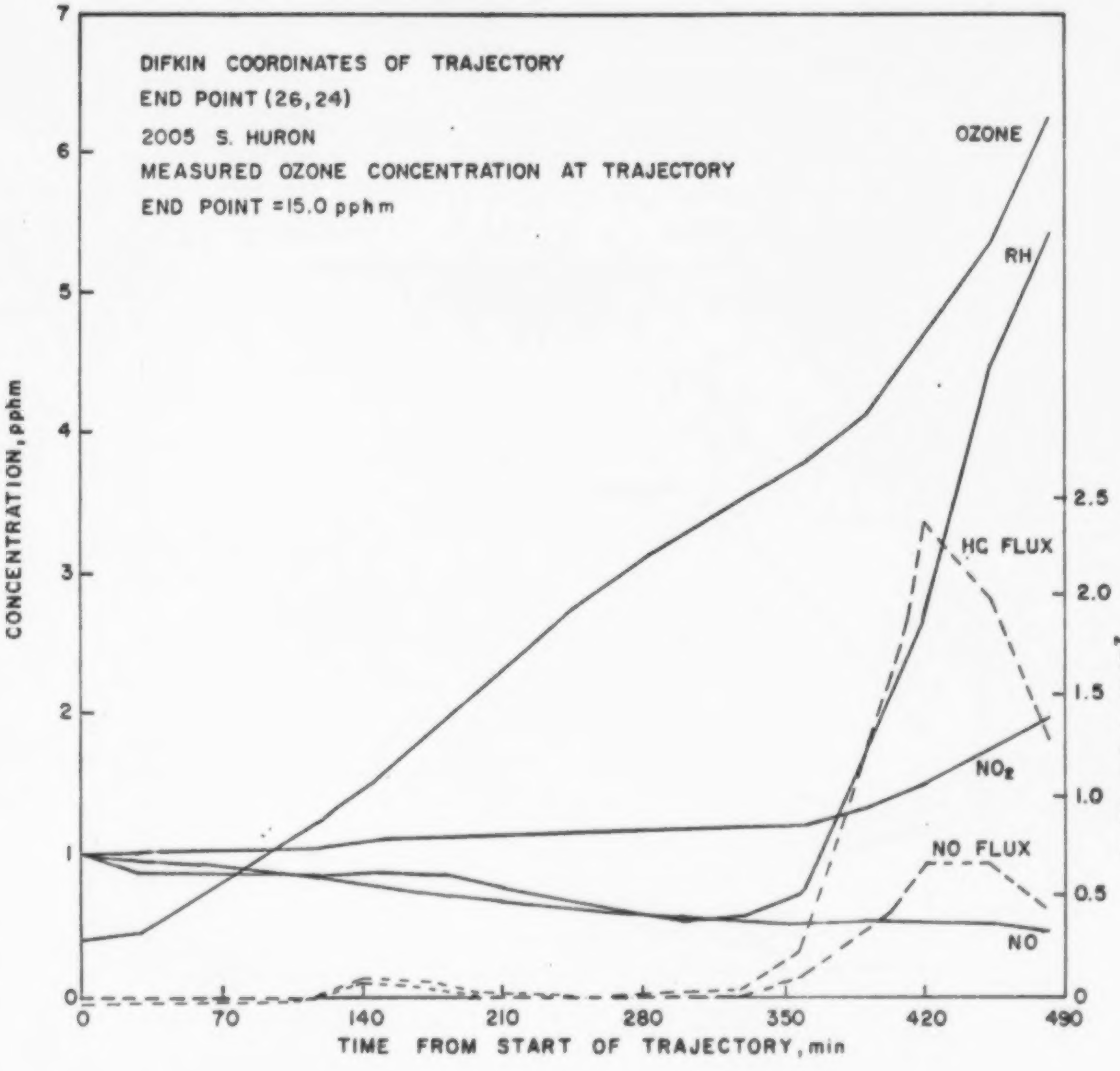

Figure 17. Fifth DIFKIN evaluation run

It is interesting that the increase of ozone with time is quite similar in the first three figures even though the pollutant fluxes along the three trajectories are quite different. A complete output listing for the first trajectory run is given in Appendix C. The first leg of the trajectory is not shown on the computer plot in Appendix C due to format restrictions. These trajectories have different durations due to the restriction that each trajectory has to originate within the DIFKIN grid. A comparison of measured and calculated CO, RH, and O_3 concentrations is shown in Table 7 for trajectories ending at 2 p.m. at each of the five measurement stations. Concentrations for RH and O_3 are consistently underpredicted. Correlation coefficients for measured and predicted concentrations are given below.

Pollutant	r
CO	0.3
HC	-0.1
O_3	-0.1

These poor correlations may be due in part to the uncertainty regarding initial pollutant concentrations and the small number of wind stations used in the trajectory determination.

EVALUATION OF THE GIFFORD-HANNA MODEL

In our discussion of the evaluation procedure for the DIFKIN model, most of the emphasis was placed on data preparation and model operating characteristics. Major modifications to the actual model structure were beyond the scope of this particular effort. For the case of the Gifford-Hanna model, however, we are actually dealing with a technique for estimating reactive pollutant concentrations, rather than a specialized photochemical model with formalized input scheme. In his description of the calculation technique, Hanna uses a set of photochemical reactions only as an example of this technique for the analysis of chemically reactive pollutants. In this case we felt that no clear distincetion could

Table 7. COMPARISON OF MEASURED AND CALCULATED CONCENTRATIONS AT 1400 HOURS FOR AUGUST 13, 1973

Station	$[\mathrm{CO}]$ calculated ppm	$[\mathrm{CO}]$ measured ppm	$[\mathrm{RH}]$ calculated pphm	$[\mathrm{RH}]$ measured pphm	$[\mathrm{O_3}]$ calculated pphm	$[\mathrm{O_3}]$ measured pphm
A	2.16	4.0	2.05	—	6.16	25.5
C	3.37	3.0	3.41	28.3	5.41	26.5
D	2.94	4.0	2.48	16.7	4.93	13.3
E	2.12	—	0.91	11.7	3.42	16.5
F	4.48	4.0	5.42	8.3	6.26	15.0

[a] The following transformation was used to convert total hydrocarbon measurements $[\mathrm{HC}]$ to reactive hydrocarbon concentrations:

$$[\mathrm{RH}]_{\mathrm{pphm}} = \frac{\dfrac{[\mathrm{HC}]\ \mu\mathrm{g/m^3\ carbon}}{665(\mu\mathrm{g/m^3\ carbon})/(\mathrm{ppm\ carbon})} - 1.5\ \mathrm{ppm\ carbon}}{6} \times 100$$

where: 665 = conversion from $\mu\mathrm{g/m^3}$ carbon to ppm carbon

1.5 ppm carbon = approximate methane background

6 = average number of carbon atoms per reactive hydrocarbon molecule

be made between minor modifications to the model or more important structural changes. Under these circumstances we felt that it was proper to present two separate evaluations of the Gifford-Hannd model. In the first procedure we modify the steady state version of the model to allow pollutant transport from adjacent grid cells. The second test involves a time-dependent model analysis of O_3, RH, and NO_x concentrations, closely following the procedure used by Hanna in his 29 September 1969 Los Angeles model validation study.

Application to Denver

In practice, the application of the Gifford-Hanna model to an area other than Los Angeles can be carried out with comparative ease due to the many simplifying assumptions made in the development of the model. It is these assumptions, however, which make the model less sensitive to the particular characteristics of a new area. For example, the Gifford-Hanna photochemical model provides no mechanism to account for variations in solar radiation intensity with latitude and elevation. The assumption that the NO_2 and NO emission rates are in the ratio of 3 to 2 is actually based upon Los Angeles concentration measurements. Furthermore, assumptions regarding the lack of cross wind variations in pollutant concentration may be more appropriate for Los Angeles than Denver. Also, as was the case for the DIFKIN model, there is no guarantee that the reaction scheme utilized in the Gifford-Hanna model validation for Los Angeles will apply in another area with a different mixture of other pollutant such as SO_2 and particulates.

Required Program Modifications - In the development of the Gifford-Hanna photochemical model the assumption was made that the atmosphere over a city could be described in terms of a single reactor volume. While such an approximation may be convenient for treating the emission, transport, and chemical transformation processes with simple expressions, it certainly restricts its application to the evaluation of those strategies which result in an overall increase of emissions over an urban area.

Spatially selective changes in emission patterns resulting from the application of transportation controls could not be studied adequately with a single box model. Hanna makes the statement in his paper[7] that his model can be easily generalized to use the advention scheme outlined in an earlier paper by Gifford and Hanna.[12] In this paper they present a method for calculating a surface concentration χ ($\mu g/m^3$) of a nonreactive substance due to area source emissions upwind of a receptor point by integration of the Gaussian plume[13] formula.

$$\chi = \int_0^D \sqrt{\frac{2}{\pi}} \frac{Q_A}{u\,\sigma_z} dx$$

where Q_A = source strength ($\mu g/m^2$-sec)
D = distance to the edge of the area source (m)
u = wind speed (m/sec)
σ_z = vertical dispersion parameter (m)
x = distance from source (m)

The vertical dispersion may be parameterized according to the following power law:

$$\sigma_z = ax^b$$

where the parameters a = 0.15 and b = 0.75 could be applied to average yearly conditions. If the receptor square (0,0) is surrounded by an array of other grid squares, then the total concentration contribution may be written as:

$$\chi = \sqrt{\frac{2}{\pi}}\; \frac{\left(\frac{\delta x}{2}\right)^{1-b}}{u\, a(1-b)} \left[Q_a(0,0) + \sum_{i=-4}^{4} \sum_{j=-4}^{4} Q_A\,(i,j) + f\,(i,j) \left[(2r+1)^{1-b} - (2r-1)^{1-b} \right] \right]$$

where $Q_A(i,j)$ = emissions from square (i,j) ($\mu g/m^2$ - s)

δx = width of a grid cell (m)

r = number of grid blocks square (i,j) is from the central square (distance)

$f(i,j)$ = parameter which depends upon the wind direction frequency distribution.

A method for mapping a radial wind direction distribution upon an array of square grid cells is illustrated in Figure 18.

For chemically reactive substances the actual concentration may be obtained by multiplying the concentration χ by the nondimensionalized value $\left[\,C\,\right]^*$. In the modified version of the Gifford-Hanna model used in this analysis, the steady state values of $\left[\,C\,\right]^*$ were obtained using the following expressions for A, Z, Δx, u and Q (variables discussed earlier).

$$A = \frac{\chi\ (i,j)\ U}{Q\ (i,j)}$$

$$Z = \frac{\Delta x}{A}$$

where Δx = distance from receptor square to square (i,j) (m)

Q = Q (i,j), the emission rate from square (i,j) ($\mu g/m^2$-sec)

$\chi\ (i,j)$ = concentration contribution due to emissions from square (i,j)

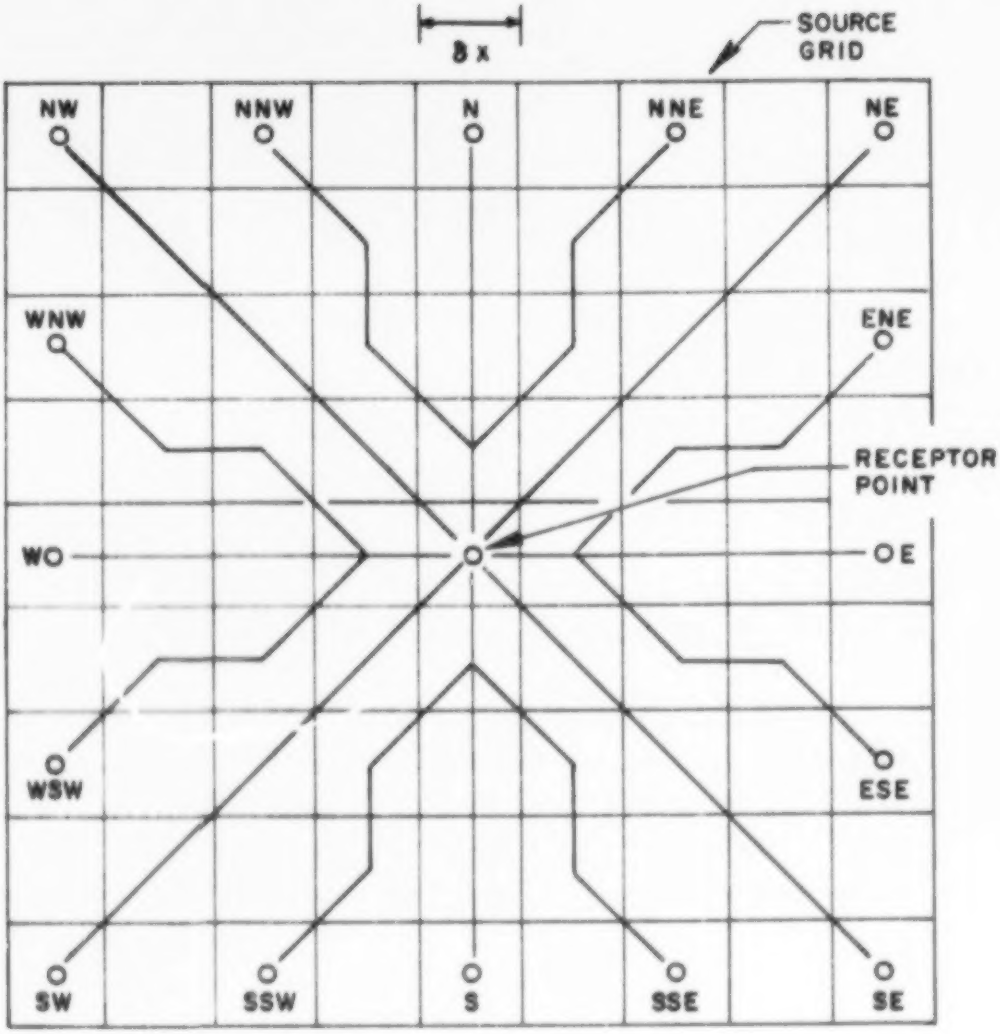
δx
SOURCE GRID
NW
NNW
N
NNE
NE
WNW
ENE
RECEPTOR POINT
W
E
WSW
ESE
SW
SSW
S
SSE
SE

Figure 18. Scheme for combining rectilinear source-grid squares with radial wind directions

APPLICATION RESULTS

Input Data Base

The required input for the Gifford-Hanna model is a subset of the data base used for DIFKIN with the exception that the Gifford-Hanna model does not calculate its own emissions from VMT data. To generate NO_x and total hydrocarbon emissions from mobile sources the methodology of AP-42[14] was employed to calculate HC and NO_x emissions for grid squares 8 mi on a side, following the procedure used in the Los Angeles validation. This emission network was constructed from the Denver APRAC-la grid (with one column of 2 mi by 2 mi dummy squares added on the east side), which was discussed in connection with the DIFKIN model input. This grid, shown in Figure 19, was utilized in our modified steady state version of the Gifford-Hanna model. These emission rates represent an average over the period from 6 a.m. to 12 noon. For the time dependent validation an emission rate for each hour was obtained from a spatial average of emission rates over a subset of six 8 mi by 8 mi squares ((1,2), (1,3), (2,2), (2,3), (3,2), (3,3)). Stationary source emissions were not input to the Gifford-Hanna model. Since the emission rates required by the model are in units of $cm^3/m^2/sec$ the g/sec emissions of HC were converted with the assumption that the molecular weight is equal to 42g. This is really an overestimate of reactive hydrocarbon emissions since it implies that the mobile source hydrocarbon emissions are 100 percent propylene. In the DIFKIN model the calculated mobile source hydrocarbon emissions were scaled by the factor 0.7 to obtain the reactive fraction. Another important difference between DIFKIN and Gifford-Hanna emission schemes is that the former model assumes that all NO_x emissions are actually NO, while the latter uses an NO/NO_2 emission ratio of 1.5.

The meteorological input for the steady state version of the Gifford-Hanna model consists of an average wind speed and direction for three meteorological stations over the period of 6 a.m. to 12 noon for the validation

```
SOURCE STRENGTHS FOR NO IN CM**3/M**2/SEC

 0.00003 0.00022 0.00007 0.00001

 0.00010 0.00090 0.00047 0.00003

 0.00006 0.00070 0.00042 0.00001

 0.00000 0.00007 0.00006 0.00001


SOURCE STRENGTHS FOR NO2 IN CM**3/M**2/SEC

 0.00002 0.00014 0.00004 0.00001

 0.00007 0.00059 0.00031 0.00002

 0.00004 0.00045 0.00027 0.00000

 0.00000 0.00004 0.00004 0.00001


SOURCE STRENGTHS FOR RH IN CM**3/M**2/SEC

 0.00006 0.00048 0.00015 0.00002

 0.00024 0.00209 0.00113 0.00006

 0.00013 0.00167 0.00099 0.00002

 0.00000 0.00017 0.00012 0.00002
```

Figure 19. Emission density pattern for steady state Gifford-Hanna model validation for Denver (6 a.m. to 12 noon average)

day. In the validation of the time dependent model hourly wind speeds from the nearest meteorological station were utilized for each hour for purposes of scaling the nondimensionalized concentrations.

This combined Gifford-Hanna multiple area source and photochemical model allows for emissions to be input from more than one grid square. In our validation studies, which will be described later, both this modified steady state and the original time-dependent version of the Gifford-Hanna model will be evaluated.

Concentration Measurements

The Gifford-Hanna model validation exercise utilized the same August 13, 1973 hourly concentration measurements that were employed in the DIFKIN model evaluation. For the steady state model validation, noon concentration measurements were compared with predicted values. In the evaluation of the time-dependent model, 6 a.m. concentrations are projected in time by 1 hour increments using wind speeds, emission rates, and nondimensionalized concentrations. These projected concentrations are then compared with actual measurements at the respective locations.

The first validation test of the Gifford-Hanna model was performed using our modified version of their approach discussed eaerlier in this section. Using this technique we generated "steady state" concentrations of NO, NO_2, HC, and ozone for an array of 16 grid squares each 8 mi on a side. An average wind speed of 1.74 m/sec from a distribution of wind directions and a neutral stability condition were assumed for this test. The results of calculations given in Figure 20 show that as in the case of DIFKIN, ozone concentrations, based upon a noon measurement, are underpredicted. Even the highest calculated ozone concentration (2.0 pphm) among the 16 squares was considerably below the average measured noon value (15.9 pphm) among all of the stations.

```
CONCENTRATIONS OF NO FROM GROUND SOURCES
0.7E-02 0.3E-01 0.1E-01 0.2E-02

0.2E-01 0.1E 00 0.6E-01 0.6E-02

0.2E-01 0.8E-01 0.5E-01 0.5E-02

0.2E-02 0.1E-01 0.1E-01 0.4E-02

CONCENTRATIONS OF NO2 FROM GROUND SOURCES
0.5E-02 0.2E-01 0.9E-02 0.1E-02

0.1E-01 0.9E-01 0.4E-01 0.4E-02

0.1E-01 0.6E-01 0.4E-01 0.3E-02

0.2E-02 0.9E-02 0.8E-02 0.3E-02

CONCENTRATIONS OF RH FROM GROUND SOURCES
0.2E-01 0.7E-01 0.3E-01 0.5E-02

0.5E-01 0.3E 00 0.1E 00 0.1E-01

0.4E-01 0.2E 00 0.1E 00 0.1E-01

0.6E-02 0.3E-01 0.3E-01 0.9E-02

CONCENTRATIONS OF O3
0.1E-01 0.1E-01 0.1E-01 0.1E-01

0.1E-01 0.2E-01 0.1E-01 0.1E-01

0.1E-01 0.2E-01 0.1E-01 0.1E-01

0.1E-01 0.1E-01 0.1E-01 0.1E-01
```

Figure 20. Concentration (ppm) profiles for steady state Gifford-Hanna model validation for Denver (August 13, 1973 - 12 noon)

The simple Gifford-Hanna photochemical model was then applied to analyze hourly concentrations from 6 a.m. to noon. In this method, almost identical to the one used by Hanna, values for A and Z were determined from Table 2 assuming neutral stability conditions. For purposes of calculation of the nondimensionalized concentrations, an average wind speed of 1.74 m/sec was used to represent the average winds during the 6 a.m. to noon period. An average emission density was obtained by averaging emissions from six adjacent grid cells with the highest emissions. These input parameters were then used to obtain hourly nondimensionalized concentrations for HC, NO, and NO_2 by solving Equations (1) through (3) using a Runge-Kutta technique and assuming all nondimensionalized concentrations are equal to 1.0 at 6 a.m. With the exception of ozone, concentrations for the period after 6 a.m. were calculated according to the following expression:

$$\left[C\right] = \frac{U_6}{U} \frac{Q}{Q_6} \left[C\right]^* \left[C\right]_6 \qquad (16)$$

where U = wind speed (m/sec)

U_6 = wind speed at 6 a.m. (m/sec)

Q = source strength ($cm^3/m^2/sec$)

Q_6 = source strength at 6 a.m. ($cm^3/m^2/sec$)

$\left[C\right]^*$ = nondimensionalized concentration

$\left[C\right]_6$ = concentration (ppm)

Ozone concentrations were determined from Equation 4 with the assumption that NO_2 and NO emissions are in the ratio of 2 to 3:

$$\left[O_3\right] = (0.02) \left(\frac{2}{3}\right) \frac{\left[NO_2\right]^*}{\left[NO\right]^*}$$

The value of the wind speed used in the determination of nondimensionalized concentrations was an average for all three meteorological stations over the period from 6 a.m. to noon. In the concentration projection described by Equation (16), the hourly wind speed measurement was taken from the meteorological site closest to the concentration measurement station. The ratio Q/Q_6 was based solely upon the hourly travel distribution used in the DIFKIN evaluation. The results of these calculations are presented in Tables 8(a) through (c), where we have compared the projected and measured values for CO, RH, and ozone. The correlations between predicted and measured concentrations are given below.

Pollutant	r
CO	0.23
RH	0.29
O_3	0.78

Although there appears to be a reasonable correlation between measured and calculated ozone concentrations, the magnitude of the calculated values is much too small for the later hours of the morning. The most interesting result of this study is that the nondimensionalized concentrations of NO, NO_2, and HC do not depart significantly from unity during the simulation period. The conclusion which may be drawn for the Gifford-Hanna calculations is that the impact of the Denver emission densities upon photochemical simulation is negligible when compared with the Los Angeles sample run.

IMPLICATIONS OF MODEL RESULTS

Although the results of our model evaluation studies were less than encouraging, we feel that there still exists a role for photochemical modeling in the 3-C planning process. In spite of the difficulties encountered in trying to achieve a reasonable agreement between measured

Table 8a. HOURLY CO VALIDATION USING SIMPLE GIFFORD-HANNA PHOTOCHEMICAL MODEL

Hour	t^*	u_6/u	Q/Q_6	$[\mathrm{CO}]^*$	$[\mathrm{CO}]$ cal	$[\mathrm{CO}]$ mea
Station A						
6	0	1.0	1.0	1.0	2.0 ppm	2.0 ppm
7	0.21	3.0	3.0	1.0	18.0	1.0
8	0.42	1.0	2.7	1.0	5.4	1.0
9	0.63	0.75	2.3	1.0	3.5	3.0
10	0.83	1.0	2.4	1.0	4.8	3.0
11	1.04	0.6	2.6	1.0	3.1	3.0
12	1.25	0.75	2.6	1.0	3.9	3.0
Station C						
6	0	1.0	1.0	1.0	2.0 ppm	2.0 ppm
7	0.21	3.0	3.0	1.0	18.0	3.0
8	0.42	1.0	2.7	1.0	5.4	2.0
9	0.63	0.75	2.3	1.0	3.5	2.0
10	0.83	1.0	2.4	1.0	4.8	2.0
11	1.04	0.6	2.6	1.0	3.1	3.0
12	1.25	0.75	2.6	1.0	3.9	4.0
Station D						
6	0	1.0	1.0	1.0	3.5 ppm	3.5 ppm
7	0.21	3.0	3.0	1.0	31.5	5.0
8	0.42	1.0	2.7	1.0	9.5	5.0
9	0.63	0.75	2.3	1.0	6.0	5.0
10	0.83	1.0	2.4	1.0	8.4	6.0
11	1.04	0.6	2.6	1.0	5.5	6.0
12	1.25	0.75	2.6	1.0	6.8	5.0

Table 8a (Continued). HOURLY CO VALIDATION USING SIMPLE GIFFORD-HANNA PHOTOCHEMICAL MODEL

Hour	t^*	u_6/u	Q/Q_6	$[CO]^*$	$[CO]$ cal	$[CO]$ mea
			Station F			
6	0	1.0	1.0	1.0	3.0 ppm	3.0 ppm
7	0.21	2.0	3.0	1.0	18.0	3.0
8	0.42	3.0	2.7	1.0	24.3	4.0
9	0.63	3.0	2.3	1.0	20.7	5.0
10	0.83	2.0	2.4	1.0	14.4	5.0
11	1.04	1.5	2.6	1.0	11.7	5.0
12	1.25	2.0	2.6	1.0	15.6	4.0

Table 8b. HOURLY RH VALIDATION USING SIMPLE GIFFORD-HANNA PHOTOCHEMICAL MODEL

Hour	t^*	u_6/u	Q/Q_6	$[RH]^*$	$[RH]$ cal	$[RH]$ mea
Station C						
6	0	1.0	1.0	1.0	35.0 pphm	35.0 pphm
7	0.21	3.0	3.0	0.99	311.9	21.7
8	0.42	1.0	2.7	0.98	92.6	18.3
9	0.63	0.75	2.3	0.97	58.6	25.0
10	0.83	1.0	2.4	0.96	80.6	28.3
11	1.04	0.6	2.6	0.96	52.4	28.3
12	1.25	0.75	2.6	0.95	64.8	46.5
Station D						
6	0	1.0	1.0	1.0	21.7 pphm	21.7 pphm
7	0.21	3.0	3.0	0.99	193.3	31.7
8	0.42	1.0	2.7	0.98	57.4	51.7
9	0.63	0.75	2.3	0.97	36.3	25.0
10	0.83	1.0	2.4	0.96	50.0	21.7
11	1.04	0.6	2.6	0.96	32.5	20.0
12	1.25	0.75	2.6	0.95	40.2	18.3
Station E						
6	0	1.0	1.0	1.0	5.0 pphm	5.0 pphm
7	0.21	3.0	3.0	0.99	44.6	5.0
8	0.42	1.0	2.7	0.98	13.2	3.3
9	0.63	0.75	2.3	0.97	8.4	3.3
10	0.83	1.0	2.4	0.96	11.5	3.3
11	1.04	0.6	2.6	0.96	7.5	5.0
12	1.25	0.75	2.6	0.95	9.3	11.7

Table 8b (Continued). HOURLY RC VALIDATION USING SIMPLE GIFFORD-HANNA PHOTOCHEMICAL MODEL

Hour	t^*	u_6/u	Q/Q_6	$[RH]^*$	$[RH]_{cal}$	$[RH]_{mea}$
Station F						
6	0	1.0	1.0	1.0	15.0 pphm	15.0 pphm
7	0.21	3.0	3.0	0.99	133.7	11.7
8	0.42	1.0	2.7	0.98	39.7	18.3
9	0.63	0.75	2.3	0.97	25.1	18.3
10	0.83	1.0	2.4	0.96	34.6	21.7
11	1.04	0.6	2.6	0.96	22.5	18.3
12	1.25	0.75	2.6	0.95	27.8	11.7

Table 8c. HOURLY O_3 VALIDATION USING SIMPLE GIFFORD-HANNA PHOTOCHEMICAL MODEL

Hour	t^*	$[O_3]$ cal	$[O_3]$ mea
Station A			
6	0	1.4 pphm	1 pphm
7	0.21	1.4	3
8	0.42	1.4	4
9	0.63	1.5	-
10	0.83	1.5	9
11	1.04	1.5	14
12	1.25	1.6	19
Station C			
6	0	1.4 pphm	2 pphm
7	0.21	1.4	3
8	0.42	1.4	5
9	0.63	1.5	6
10	0.83	1.5	11
11	1.04	1.5	16
12	1.25	1.6	21
Station D			
6	0	1.4 pphm	1 pphm
7	0.21	1.4	3
8	0.42	1.4	9
9	0.63	1.5	6
10	0.83	1.5	-
11	1.04	1.5	12
12	1.25	1.6	16

Table 8c (Continued). HOURLY O_3 VALIDATION USING SIMPLE GIFFORD-HANNA PHOTOCHEMICAL MODEL

Hour	t^*	$[O_3]$ cal	$[O_3]$ mea
		Station E	
6	0	1.4 pphm	3 pphm
7	0.21	1.4	-
8	0.42	1.4	4
9	0.63	1.5	5
10	0.83	1.5	6
11	1.04	1.5	8
12	1.25	1.6	12
		Station F	
6	0	1.4 pphm	-
7	0.21	1.4	3 pphm
8	0.42	1.4	3
9	0.63	1.5	6
10	0.83	1.5	13
11	1.04	1.5	16
12	1.25	1.6	11

and calculated concentrations, the two models used in this study can provide some degree of insight into the relationship between ozone and NO_x concentrations and emissions and meteorological parameters. It is hoped, however, that before further model applications are carried out, a much greater effort be expended in applying and validating these models for other urban areas besides Los Angeles. In light of the problems we encountered in the application of these models to just a single city, we feel that an effort of this type would certainly be worthwhile. In this connection we recommend that more attention be devoted to the selection of reasonable initial concentrations for the air parcels and that a greater number of meteorological stations be used for the determination of trajectories, if possible.

It must be emphasized that during this modeling exercise we did not set out to conduct an extensive theoretical evaluation of the technical aspects of each model. Such activities would have been beyond the scope of this particular effort. Rather, we have assumed the role of a 3-C planning agency in our approach to these models so that our findings relate as much to the general feasibility of model application as well as to the accuracy of the calculation technique. This is why we have devoted a considerable section of this report to the treatment of the more logistical aspects of model application such as data collection and validation procedures. Where appropriate, we have called out what we felt to be significant technical flaws in the models. An example is the problem we found in selecting initial pollutant concentrations for the DIFKIN model. It is hoped that the experiences we have described will be of value to other photochemical modeling applications.

REFERENCES

1. Reynolds, S. D., Mei-Kao Lui, T. A. Hecht, P. M. Roth, and J. H. Seinfield. Urban Air Shed Photochemical Simulation Model Study. Volume I - Development and Evaluation. Prepared by Systems Applications, Inc., Beverly Hills, California for the Office of Research and Development. U. S. Environmental Protection Agency. Washington, D. C. EPA-R4-73-030a. July 1973.

2. Reynolds, S. D. Urban Air Shed Photochemical Simulation Model Study. Volume II - User's Guide and Description of Computer Programs. Prepared by Systems Applications, Inc., Beverly Hills, California for the Office of Research and Development. U. S. Environmental Protection Agency. Washington, D. C. EPA-R4-73-030f. July 1973.

3. Wayne, L. G., A. Kokin, and M. I. Weisburd. Controlled Evaluation of the Reactive Environmental Simulation Model (REM). Volume I: Final Report. Prepared by Pacific Environmental Services, Inc. Santa Monica, California for Office of Research and Monitoring Environmental Protection Agency. Washington, D. C. EPA R4-73-013a. February 1973.

4. Kokin, A., L. G. Wayne, and M. Weisburd. Controlled Evaluation of the Reactive Environmental Simulation Model (REM). Volume II: User's Guide. Prepared by Pacific Environmental Services, Inc. Santa, Monica, California for the Office of Research and Monitoring. Environmental Protection Agency. Washington, D. C. EPA R4-73-013b. February 1973.

5. Eschenroeder, A. Q., J. R. Martinez, and R. A. Nordsieck. Evaluation of a Diffusion Model for Photochemical Smog Simulation. Prepared by General Research Corporation. Santa Barbara, California for the Environmental Protection Agency. EPA-R4-73-012, Volume a. October 1972.

6. Martinez, J. R., R. A. Nordsieck, and M. A. Hirschberg. User's Guide to Diffusion/Kinetics (DIFKIN) Code. Prepared by General Research Corporation. Santa Barbara, California for the Environmental Protection Agency. EPA-R4-73-012, Volume b. December 1973.

7. Hanna, S. R. A Simple Dispersion Model for the Analysis of Chemically Reactive Pollutants. Atmospheric Environment. Pergamon Press. 7:803-817. 1973.

8. Friedlander, S. K. and J. H. Seinfeld. A Dynamic Model of Photochemical Smog. Environmental Science and Technology. 3:1175-1181. 1969.

9. Stanford Research Institute. User's Manual for the APRAC-1A Urban Diffusion Model Computer Program. Prepared for the Coordinating Research Council and the United States Environmental Protection Agency, Division of Meteorology. September 1972.

10. Refinement and Modification of Planning Models and Techniques. Calibration of the Existing Highway Network for the Denver Metropolitan Area. Colorado Division of Highways. Planning and Research Division. Joint Regional Planning Program Technical Memorandum 4-2/001. October 1973.

11. Martinez, J. R., R. A. Nordsieck, and A. Q. Eschenroeder. Morning Vehicle-Start Effects on Photochemical Smog. Environmental Science and Technology.

12. Gifford, F. A., Jr. and S. R. Hanna. Modeling Urban Air Pollution. Atmospheric Environment 7:131-136. 1973.

13. Gifford, F. A., Jr. An Outline of Theories of Diffusion in the Lower Layers of the Atmosphere. Chapter 3. Meteorology and Atomic Energy 1968 (D. Slade, editor,) USAEC-TID-24190. 1968.

14. Compilation of Air Pollutant Emission Factors, Second Edition. U. S. Environmental Protection Agency. Office of Air and Water Programs. Office of Air Quality Planning and Standards. Research Triangle Park, North Carolina. April 1973.

SECTION V

CASE STUDY OF AIR QUALITY REVIEW REQUIREMENTS

GENERAL

This Section will present a case study of some of the present requirements for reviewing the air quality impacts of highway systems. Two specific examples will be examined:

1. Review of urban transportation plans and programs for consistency with State Implementation Plans ("109(j) review").
2. Evaluation of major highways for oxidants impact under EPA indirect source review regulations.

Both examples are drawn from the Denver transportation planning process. In both cases, oxidants are the concern, not other pollutants. Review requirements studied here were those in effect when this project began and many have subsequently been revised.

The following discussion will begin with the consistency review, followed by the indirect source review, and then by some concluding remarks.

CONSISTENCY REVIEW

Introduction

Requirements - Section 109(j), Title 23 USC (added by Section 136(b) of the Federal-Aid Highway Act of 1970, P.L. 91-605) states that:

> "the Secretary, after consultation with the Administrator of the Environmental Protection Agency, shall develop and promulgate guidelines to assure that highways constructed pursuant to this title are consistent with any approved plan for the implementation of any ambient air quality standard for any air quality control region designation pursuant to the Clean Air Act, as amended."[1]

The Federal Highway Administration (FHWA) has promulgated guidelines as required by the law quoted above. Interim guidelines were issued in 1973,[2] followed by revised, final guidelines in late 1974.[3] An Environmental Impact Statement[1] was prepared on the final (1974) guidelines.

The present analysis will use the 1973 guidelines which were in effect at the start of this project.

Under the 1973 FHWA guidelines, the highway agency is required to:

> "establish a continuing review procedure with the cognizant air pollution control agency to:
>
> "(i) Assess the consistency of the transportation plan and program with the approved State Implementation Plan;
>
> "(ii) Annually solicit comments from the cognizant air pollution control agency including its assessment of the consistency of the plan and program with the approved State Implementation Plan prior to plan approval by the policy board.
>
> "(iii) Identify and resolve differences with the cognizant air pollution control agency."

An annual determination of consistency between the transportation plan and the State Implementation Plan (SIP), often referred to as the "109(j) review," must be documented and endorsed by the 3-C* agency policy board. The guidelines require that both the highway plans and the planning process be reviewed for consistency, and that the FHWA Regional Administrator must consult with the EPA Regional Administrator in these reviews. This review for consistency is one of many items that FHWA required be done to obtain the annual certification of each agency's 3-C planning process.

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*"3-C" refers to the continuing, comprehensive, cooperative transportation planning process required by 23 USC, Section 134.

The guidelines also specify that a particular highway project cannot be approved unless the FHWA determines that it is consistent with the SIP. This project determination is to be included in the environmental impact statement for the highway project.

Example of Consistency Review - In the discussion to follow, an example will be presented of how the 109(j) consistency review would proceed, using the Denver 3-C planning as a case study. In this example, what will be examined is how EPA would participate, not how FHWA would perform its review. Hence, the intent is to perform a trial run of the existing requirements and guidelines.

Criteria for EPA Review

The FHWA guidelines cited above require that the FHWA and EPA Regional Administrators consult with one another at certain times and that the EPA identify deficiencies to the FHWA. However, the FHWA guidelines (including the later 1974 revision) provide no criteria nor identify any technical methods for the EPA functions.

EPA had not (as of the start of this project) formally established any procedures or criteria for its role. EPA is expected, however, to issue guidance on consistency review shortly.[*] In the interim, certain tentative procedures or guidelines[4] have been recommended to the EPA Regional Administrators. These instructions, referred to as the Strelow-Myers Memo, will be used here as the basis for the example consistency review.

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[*] This has been issued as "Guidelines for Analysis of Consistency Between Transportation and Air Quality Plans and Programs," prepared jointly by EPA and FHWA, April, 1975.

Another possible source of guidance for EPA review of 109(j) consistency is suggested by EPA[4] to be a report[18] prepared by a consultant as part of the guidelines for air quality maintenance planning. Because the report was not final before the present project was begun, it will only be used as a reference and not as if it were a formal basis for review.

The Denver Situation

Status of the 3-C Process - The 3-C transportation planning process in the Denver metropolitan area is carried out jointly by the Colorado Division of Highways (CDH), the Regional Transportation District (RTD), and the Denver Regional Council of Governments (DRCOG). This is referred to as the Joint Regional Planning Program (JRPP). The JRPP has just produced its official long-range transportation plan[5] for the Denver region, and it is presently developing a program for implementing the plan. The plan is for the year 2000. No schedules have yet been adopted for construction of either the highway element or the public transportation element. In the lexicon of 3-C planning, the JRPP is now in Phase IV, implementation and continuing planning.

Plans - For this trial evaluation, the JRPP will be evaluated primarily on the basis of the following of its products:

- The year 2000 transportation plan, as described in the report of the adopted plan[5] and the technical analysis.[6]
- The draft short-term plan[7] available when this project began.
- The current operations plan[8] for the JRPP.

This review has been based upon information available in the fall of 1974 and may not accurately reflect the current status of the JRPP. The actual 109(j) review and certification of the JRPP is still underway; FHWA, EPA, and the other agencies involved have not yet reached agreement on whether 109(j) requirements are being met and certification has not yet been granted.

Colorado State Implementation Plan - In order to assess the 3-C plan and program it is necessary to compare it with pertinent elements of the State Implementation Plan (SIP).

GCA reviewed the SIP, and its Transportation Control Plan (TCP) component, in a previous report.[9] There it was found that the promulgated TCP includes several elements:

1. Program for inspection and maintenance of motor vehicles, using the idle test mode, to be fully implemented by 1 December 1975.
2. Program for equipping of pre-1968 model year vehicles with engine air bleed devices, to be implemented by 1 July 1976.
3. Program for modification of 1968-1975 model year vehicles for high altitude, to be implemented by 1 July 1976.
4. Program for control of hydrocarbon emissions from stationary transportation, manufacturing, and processing facilities.
5. Creation of bus-carpool lanes on existing roadways.
6. Limitation on construction of parking facilities, to be implemented on 1 January 1975.
7. Removal of on-street parking in the Denver Central Business District (CBD).
8. Mass transit improvements.
9. Limitation on gasoline sales.

EPA Region VIII now expects the TCP to be amended to include slightly different measures for inspection and maintenance and for modification of existing automobile engines.

In response to the EPA-promulgated TCP, the Air Pollution Control Commission (APCC) recently promulgated Regulation number 9 which deals explicitly with measures 5 through 8 mentioned above. Elements of Regulation number 9 are:

1. Exclusive Bus-Carpool Lanes, to be implemented by 1 January 1976.

2. Creation of Park-N-Ride Facilities with Express buses to the CBD; with plan submission by 1 October 1974.

3. Carpooling programs, to be implemented by large employers (>250 employees) by 1 April 1975, and by other employers (50 to 250 employees) by 1 October 1975. In addition, employers must submit a description of incentives which encourage employees to make use of mass transit facilities. Large employers must submit their plan by 1 February 1975, with submittal by other employers by 1 August 1975.

In addition, the regulation requires that DRCOG submit recommendations to the APCC by 1 March 1975 on parking requirements that may stimulate the use of public transportation and decrease single passenger VMT.[9]

The RTD is specifically charged with planning the details of the bus-carpool lanes and park-and-ride facilities.

These SIP elements will be the basis for consistency evaluation.

Consistency Review of 3-C Plans

An urban transportation planning process is complex, involving numerous activities and people. Consequently it is difficult to assess except by examining its products. Nonetheless there are some other indicators that can be examined. One is the operations plan, which is intended to be a description of the long range planning activities of the JRPP. Review of the current operations plan[8] shows that there are repeated references to air quality, but only as one of many nontransportation considerations in the 3-C process. In its description of the JRPP organization, no specific provisions are made for formally incorporating air quality planning. As an example, the Colorado Air Pollution Control Commission is not identified as one of the official participants in plan preparation or review. Neither

EPA guidelines[4] nor FHWA guidelines[2] for 109(j) review define how to ensure that air quality is considered in the planning process, nor does the approved SIP mandate any specific role in transportation planning for the air agencies. Nonetheless, this would appear essential for a formal arrangement for coordination and cooperation between the air pollution control agency and JRPP. This apparent deficiency has also been cited by the Colorado Air Pollution Control Commission.[10]

Although evidence of such formal coordination is not apparent from the present review, the JRPP does claim to have established coordination. In its own presentation relative to the 109(j) review, the JRPP Agency Directors stated:

> "The Colorado Department of Highways has established a continuing review procedure with the Air Pollution Control Division of the Colorado Department of Health to assess the consistency of each project with the State Implementation Plan for air quality.
>
> "The Colorado Department of Highways is presently developing an acceptable modeling technique for analyzing air quality impacts on a regional basis. This model will be used by the Joint Regional Planning Program to assess its long range and short range transportation plans and programs."[11]

In conclusion, it is not clear from this review whether there is adequate coordination between the JRPP and the air agency. An appropriate determination would require more formal arrangements for incorporation of air quality considerations in transportation planning before certifying 109(j) compliance.

Consistency Review of Long-Range Plans

EPA's guidance on 109(j) review calls for concentrating on short-term plans, with the idea of examining long-range projects after air quality maintenance planning is underway. Denver's long-range plans will nonetheless be reviewed briefly here, because a demonstration air quality maintenance plan has been done for Denver,[9] and the short-range plan[7] is not yet well defined.

First, the long-range plan[5] does not explicitly provide for all the specific SIP measures listed earlier (e.g., bus-carpool lanes). It is not intended to be a detailed design of any facility, so this might not be judged to be a deficiency. Second, the long-range plan does explicitly include a major increase in the public transportation system. GCA earlier analyzed the JRPP plan and showed that in 1985, at the end of the air quality maintenance forecasting period, the JRPP plan would reduce total vehicle-miles of travel by an estimated 6 percent compared to an alternative highway-intensive plan. No specific computation was made of emissions for the two cases; automotive exhaust emissions would presumably be lower with the JRPP plan. Furthermore, it was estimated (on the basis of linear rollback) that in 1985 the regional ambient concentrations of carbon monoxide and oxidants would meet national standards.[9]

While there are many issues beneath these simple statements, it is reasonable to conclude that the analysis done to date does not indicate that the long-range JRPP plan would be inconsistent with the SIP in the long run. No analysis has been done to demonstrate the oxidants impact of the proposed plan relative to any alternative plan, however.

Consistency Review of Short-Term Plans

At present the JRPP short-range plan[7] deals only with a 5-year highway plan. Public transportation elements are being planned in conjunction with JRPP by one of its members, the Regional Transportation District, but separate short-range plans are being prepared. As was noted earlier, RTD is preparing plans for complying with the transit-related elements of the SIP. The short-range highway plan could nevertheless be faulted for not mentioning either the exclusive bus-carpool lanes or the park-and-ride facilities. Furthermore, the draft short-term plan explicitly states that selection of projects has been on the basis of transportation need, without apparent explicit regard for air quality.

To assess the air quality implications of the short-range plan would require an air quality analysis of each major project proposed for the 5-year period. The only such analysis reviewed for the present study is the macroscale analysis in the maintenance study.[9] It is not possible from that analysis to state whether one or more of the proposed projects would either delay attainment or cause a violation of the air quality standards. Furthermore, no such analysis can be made without a comparison of the traffic flows with and without the proposed projects. No traffic projections have been done yet for the short-term plan; the projections[6] have been done only for the year 2000, with no intermediate forecasts. The intermediate year forecasts, in turn, cannot be done until intermediate year constructions programs are tentatively agreed upon, which was just being done as the present review was begun. Without such traffic analyses it is not possible quantitatively to state the impact on regional air quality of the 5-year highway program or any element thereof.

The conclusion, then, is that the short-range highway plan requires further development and air quality analysis before consistency can be assessed. It might thus be argued that certification should be granted on the basis that no inconsistencies are apparent and that the planning work cannot continue without certification.

INDIRECT SOURCE REVIEW

Introduction

An example indirect source review was performed in order to determine the ability of the present requirements and procedures to assess the impact of major highway projects on oxidant concentrations.

Requirements

At the time this project began, EPA had published regulations[12] for the review of the air quality impact of highways and other "indirect sources" of air pollution.* The regulations focused on carbon monoxide, but specified that oxidants review would be required for highways with more than 50,000 vehicles per day within 10 years of construction.[13] Detailed guidelines[14] have been provided for the analysis required by the regulations. The guidelines, like the regulations, deal chiefly with carbon monoxide but include a brief procedure for the analysis of oxidant impacts. The review reported here used the oxidants procedure[15] from the guidelines.

Case Study

Three highways in the Denver transportation system plan[5] are expected to carry a volume of 50,000 vehicles per day or more and thus would be required to be reviewed for oxidants under current guidelines. (One of these three, I-470, is a major new highway in an underdeveloped corridor in the southwest Denver area and was previously studied for this project in connection with the DIFKIN model described in Section IV of this report). An analysis was performed of a highway of the general type to be built in all three cases: divided highways with an Average Annual Daily Traffic of 50,000. It was determined from telephone conversations with officials of the Colorado Division of Highways that enough design information would be available for any of the three highways to perform the requisite analysis.

Calculations were performed to determine the rate of emissions of both hydrocarbons and nitrogen oxides from the generalized highway. Performance of the calculations was straightforward.+ At the conclusion of the calculations, the procedure calls for comparison of the emissions from the highway with those that would occur without the highway.[16] However, no guidance is given for establishing a reference geographic area, so that the comparison will be quite different depending upon what size of area is chosen.

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*The implementation of these regulations was later delayed but technical requirements have not been altered.

+Certain steps could be clarified in the procedure.[15] In particular the procedures do not clearly identify how to treat traffic flows in the two directions.

An alternative guideline document is one used for review of environmental impact statements.[17] Again, this document is a nonbinding guideline for internal EPA use. This guideline includes a brief procedure for a mesoscale analysis for HC and NO_x, but again gives little guidance on how to select the appropriate geographic area for the analysis.

In conclusion, existing EPA guidelines do not provide sufficient guidance to allow a quantitative assessment of the oxidants impact of an indirect source (in this case, a highway).

SUMMARY AND CONCLUSIONS

The example review of the Denver area 3-C planning process and plan has shown that:

1. More formal arrangements must be made to assure consideration of air quality in JRPP transportation planning.
2. The long-range JRPP plan has been analyzed by linear rollback techniques and appears to be acceptable for maintaining air quality, but no quantitative air quality comparison has been made between the proposed plan and any alternative.
3. The short-range plan, a part of the long-range plan, is not adequately documented but shows no qualitative inconsistencies with the SIP. On the other hand, no air quality analysis has been performed to show whether some or all of the short-range projects would delay attainment of the ambient air quality standards. Hence, it is not possible to assess its consistency with the intent of the SIP to attain the standards, regardless of whether the system would allow meeting standards when completed. It might be argued, however, that the planning process should be certified so that the necessary planning and analysis can proceed.

With respect to indirect source review, it was found that present EPA mesoscale evaluation procedures do not provide adequate guidance for evaluation of the oxidants impacts of highways, one reason being the difficulty of defining the geographic area to be used for evaluations.

In summary, present guidance does not provide the procedures or methods necessary for deciding whether either entire highway systems or component projects are consistent with air quality goals. In particular, present processes for consistency review of transportation system plans would require the addition of a qualitative air quality review to allow determination of consistency with the SIP.

REFERENCES

1. Final Environmental Impact Statement. Air Quality Guidelines. U.S. Department of Transportation, Federal Highway Administration, Washington, D.C. Report Number FHWA-EIS-73-01-F. September 1974. p. 1, 17-21.

2. Air Quality Guidelines. U.S. Department of Transportation, Federal Highway Administration, Washington, D.C. Federal-Aid Highway Program Manual. Volume 7, Chapter 7, Section 9. (Also published in Fed Register. Vol. 38, November 16, 1973. pp. 31677-31679).

3. Air Quality Guidelines. U.S. Department of Transportation, Federal Highway Administration, Washington, D.C. Federal-Aid Highway Program Manual. Volume 7, Chapter 7, Section 9. Transmittal 105, November 26, 1974. Total pages: 11. (Also published in Fed Regist, Vol. 39, December 24, 1974. pp. 44441-44443.)

4. Acting Assistant Administrator for Air and Waste Management, and Director, Office of Federal Activities, U.S. EPA. Coordinated Procedures for Review of Highway Air Quality Impacts. Memorandum of All Regional Administrators. U.S. Environmental Protection Agency. Washington, D.C. PG-E-74-1. April 26, 1974. 8 pages (plus attachments).

5. Denver Regional Council of Governments. Regional Land Use, Highway and Public Transportation Plans/Denver Region. Summary Report. Draft. October 17, 1973.

6. Denver Regional Council of Governments. Transportation System Report. December 1973.

7. Denver Regional Council of Governments. Transportation Systems Planning. A Five Year Capitol Improvement Program. June 30, 1974. Draft.

8. Joint Regional Planning Program. Joint Regional Planning Program Operations Plan. Revised, October 1974.

9. GCA/Technology Division. Development of an Example 10-Year Air Quality Maintenance Plan for Denver AQMSA. Final Report. Prepared for U.S. Environmental Protection Agency, Research Triangle Park, N. C. 27711. September 1974.

10. Colorado Department of Health, Colorado Air Pollution Control Commission. Letter to Mr. David Howell, Denver Regional Council of Governments. April 1, 1974. Enclosure: Consistency Assessment.

11. Joint Regional Planning Program Assessment Statement. Enclosure to: Colorado Department of Highways. Letter to Mr. A. J. Siccandi, Division Engineer, Colorado Division, Federal Highway Administration. May 7, 1974.

12. U.S. Environmental Protection Agency. Review of Indirect Sources. 40 CFR, Part 52.22(b). In: 39 FR 25292ff. July 9, 1974.

13. Ibid, Part 52.22(b)(6)(iii).

14. Guidelines for the Review of the Impact of Indirect Sources on Ambient Air Quality. U.S. Environmental Protection Agency, Research Triangle Park, N. C. 27711. Draft. January 1975.

15. Ibid. Appendix A, Methods for Estimating Emissions From Highways.

16. Ibid. p. A-3.

17. Guidelines for Review of Environmental Impact Statements. Volume 1. Highway Projects. U.S. Environmental Protection Agency, Office of Federal Activities. September 1973. pp. 27, 28.

18. Guidelines for the Review of Urban Transportation Plans and Programs Pursuant to 23 CFR 770.204. Draft Report. Alan M. Voorhees and Associates, Inc. EPA Contract 68-02-1388. April 1974.

APPENDIX A

BLOCK DATA FOR DIFKIN RUN

```
0001             BLOCK DATA
          C
          C          BLOCK DATA PROGRAM NUMBER  ONE
          C
          C          LOAD TRAFFIC AND STATIONARY SOURCE DATA INTO COMMON /DATFIL/
          C
0002             COMMON /DATFL1/ FFWY(25,25), FSRF(25,25), FXNO2(25,25),
                1                FXHCR(25,25), FPPNO2(30,3), FORNO2(30,3),
                2                FORHCR(30,3)
0003             DIMENSION FFWYA(385), FFWYB(240), FSRFA(264), FSRFB(163),
                1          FSRFC(154), FSRFD(44), FXNO2A(291), FXNO2B(174),
                2          FXNO2C(160), FXHCRA(290), FXHCRB(172), FXHCRC(163)
0004             EQUIVALENCE (FFWYA(1),FFWY(1,1)), (FFWYB(1),FFWY(11,16)),
                1              (FSRFA(1),FSRF(1,1)), (FSRFB(1),FSRF(15,11)),
                2              (FSRFC(1),FSRF(3,18)), (FSRFD(1),FSRF(7,24)),
                3              (FXNO2A(1),FXNO2(1,1)), (FXNO2B(1),FXNO2(17,12)),
                4              (FXNO2C(1),FXNO2(16,19)), (FXHCRA(1),FXHCR(1,1)),
                5              (FXHCRB(1),FXHCR(16,12)), (FXHCRC(1),FXHCR(13,19))
0005             DIMENSION IPPNO2(30), JPPNO2(30), XPPNO2(30),
                1          IORNO2(30), JORNO2(30), XORNO2(30),
                2          IORHCR(30), JORHCR(30), XORHCR(30)
0006             EQUIVALENCE (IPPNO2(1),FPPNO2(1,1)), (JPPNO2(1),FPPNO2(1,2)),
                1              (XPPNO2(1),FPPNO2(1,3)), (IORNO2(1),FORNO2(1,1)),
                2              (JORNO2(1),FORNO2(1,2)), (XORNO2(1),FORNO2(1,3)),
                3              (IORHCR(1),FORHCR(1,1)), (JORHCR(1),FORHCR(1,2)),
                4              (XORHCR(1),FORHCR(1,3))
          C
          C
0007             DATA FFWYA/
                &  13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,
                &  13*000.,13*000.,13*000.,13*000.,13*000.,
                &  9*000., 26.,16*000.,
                &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0., 35.,  0.,  0.,  0.,  0.,
                &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                &  0.,  0.,  0.,  0.,  0.,  0.,  0., 50.,  0.,  0.,  0.,  0.,  0.,
                &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  4.,  7.,
                &  0.,  0.,  0.,  0.,  0., 87.,  7.,  0.,  0.,  0.,  0.,  0.,  0.,
                &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  7., 28.,
                & 47., 66., 36., 54.,106., 20., 15.,  0.,  0.,  0.,  0.,  0.,  0.,
                &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                &  0., 76.,143., 28.,  0., 24.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0., 66., 68.,100.,141.,176.,
                &169.,  0.,  0.,  0., 21.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                &  0.,  0.,  0.,  0.,  0.,  1., 25., 17.,  9.,  0.,  0.,174.,  0.,
                &  0.,  0.,  0., 22.,  0.,  7., 12.,  0.,  0.,  0.,  0.,  0.,  0.,
                &  0.,  0.,  0.,  0.,  0., 24., 28., 72., 66., 67.,169.,357.,130.,
                & 97., 89., 54., 23.,  9.,  0.,  0.,  0.,  0.,  0.,  0.,
                &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  9./
```

```
0008                DATA FFNYB/
                   & 43.,  0.,208., 94., 44.,  0.,  0.,  0.,  0.,  0.,  0..  0.,  0.,
                   &  0.,  0.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0., 59.,248.,
                   & 83., 37.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  8., 53., 14.,108.,  0.,
                   & 54.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0., 21., 61.,  0., 78.,  0.,  7.,
                   & 45.,  6.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0.,  0.,  0., 81.,  0.,  0., 48.,  0.,  0., 16.,
                   & 22.,  9.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0., 45.,  2.,  0.,  0., 43.,  0.,  0.,  0., 28.,
                   & 10.,  5.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,
                   &  0.,  0.,  0.,  0.
                   &/
              C
0009                DATA FSRFA/
                   &  13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0.,  8.,  0.,  3.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0., 24.,  4.,  9.,  0.,  0.,  0.,  0.,  0.,  0.,  6.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0., 10., 31., 25., 15., 14.,  4.,  1.,  0.,  8.,  2.,  0.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0., 20., 23., 50., 78., 57., 27., 20., 10., 16.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  5.,
                   & 27., 18.,153.,139., 64., 28., 23.,  4.,  3.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  3.,  6., 23., 77.. 80.,278.,
                   &128.
                   &/
0010                DATA FSRFB/
                   & 87., 54., 15.,  1.,  0.,  1.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  2., 23., 84.,165.,174.,313.,
                   &262.,144., 63., 10.,  2.,  0.,  1.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  0.,  0., 10.,  7., 42.,109.,205.,236.,438.,299.,
                   &146., 99., 64., 14.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0.,  2., 38., 40., 66.,171.,252.,256.,633.,400.,262.,
                   &206.,117., 29., 10.,  3.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  0., 22., 15., 37.,102.,227.,269.,202.,210.,134., 22.,
                   & 51., 10.,  2.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  0.,  5., 13., 30.,113.,147.,100., 82., 51., 42., 14.,  2.,
                   &  3.,  1.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                   &  0.,  7.,  7.,  6., 30., 92.,133.,106., 38., 61.,  7.,  3.,  0.,
                    &  1.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.
                    &/
0011                 DATA FSRFC/
                    &  0.,  0.,  0.,  6.,  2.,  8.,  2.,  3., 34., 61.,102., 39., 13.,
                    &  6.,  0.,  0.,  1.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  7.,  2.,  7.,  6.,  4., 12., 29.,103.,
                    & 15.,  9.,  7.,  6.,  0.,  1.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  6.,  3.,  4.,  5., 33., 26., 18., 32., 10.,
                    &  2.,  4.,  2.,  5.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  8., 20.,  0.,  2.,  0.,  1.,  0.,
                    &  1.,  2.,  6.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.
                    &/
0012                 DATA FSRFD/
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0./
              C
              C
0013                 DATA FXNO2A/
                    &  13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,
                    &  13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,
                    &  0., 11.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  1.,  0.,  3.,  0.,  0.,  0.,
                    &  0.,  0.,  0.
                    &/
0014                 DATA FXNO2B/
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  1.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,544.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                    &  0.,  0.,  0.,  0.,  0.,  0., 65.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  4.,
                         &  0.,  8.,  0.,  1.,154.,  3., 25.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0., 51.,  2.,
                         &  0.,  0.,  0.,  3.,  9.,  0.,  4.,  0.,  8.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  1.,  2.,  0.,  0.,  3., 25.,  4.,  0.,  4.,
                         &  0.,  0.
                         &/
0015                      DATA FXNO2C/
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  1.,369., 96.,  0.,  0.,
                         & 25.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0., 12.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  4.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  4.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  3.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  1.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.
                         &/
                 C
0016                      DATA FXHCKA/
                         &  13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,
                         &  13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,13*000.,
                         &  0.,  9.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.
                         &/
0017                      DATA FXHCRB/
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  4.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  3.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0., 10.,  3.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,204.,  0.,  0.,  0.,  0.,  0.,  0.,
                         &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  8.,
                           &  0.,  1.,  0.,  0., 51.,  3.,  8.,  0.,  8.,  0.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,133.,  2.,
                           &  0.,  0.,  0.,  1., 77.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0., 58.,  1.,  0.,  2.,  2., 22.,113., 12.
                           &/
0018                        DATA FXHCRC/
                           & 25.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0., 21., 13.,249.,  0.,  0.,
                           & 13.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0., 13.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0., 66.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  1.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
                           &  0.,  0.,  0.,  0.,  0.,  0.,  0.
                           &/
                      C
0019                        DATA IPPNO2/30*0/
0020                        DATA JPPNO2/30*0/
0021                        DATA XPPNO2/30*0./
                      C
0022                        DATA IORNO2/30*0/
0023                        DATA JORNO2/30*0/
0024                        DATA XORNO2/30*0./
                      C
0025                        DATA IORHCR/30*0/
0026                        DATA JORHCR/30*0/
0027                        DATA XORHCR/30*0./
                      C
0028                        END
```

```
0001             BLOCK DATA
            C
            C        BLOCK DATA PROGRAM NUMBER  TWO
            C
            C
0002             COMMON /DATFL2/ FSLOW(25,25,4)
0003             DIMENSION FSLOW6(625). FSLOW7(625), FSLOW8(625), FSLOW9(625)
0004             EQUIVALENCE (FSLOW6(1),FSLOW(1,1,1)), (FSLOW7(1),FSLOW(1,1,2)),
                1            (FSLOW8(1),FSLOW(1,1,3)), (FSLOW9(1),FSLOW(1,1,4))
            C
0005             DATA FSLOW6/
                &130*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                & 0., 0.,55.,55., 0., 0., 0., 0., 0.,55.,55., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0.,55.,55.,55.,50.,35.,45.,50.,35.,35., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0.,45.,50.,55., 0.,45., 0., 0., 0.,10*0.,
                & 0.,55.,50.,45.,35.,30.,35.,40., 0., 0., 0.,55., 0., 0., 0.,10*0.,
                &55.,55.,55.,55., 0., 0.,40., 0., 0., 0., 0.,50., 0.,55.,55.,10*0.,
                & 0.,55.,55.,50.,50.,45.,40.,40.,40.,50.,50.,55.,55.,55., 0.,10*0.,
                & 0., 0., 0., 0.,50.,45., 0.,40.,50.,50., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0.,50.,50.,50.,50., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,50.,50.,45.,50., 0.,50., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,55.,55., 0.,55., 0.,50.,50.,55., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,55., 0., 0.,55., 0., 0.,50.,50.,55., 0., 0.,10*0.,
                & 0., 0., 0.,55.,55., 0., 0.,55., 0., 0., 0.,50.,50.,50., 0.,10*0.,
                &95*0./
            C
0006             DATA FSLOW7/
                &130*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,50., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,50., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,50., 0., 0., 0., 0.,10*0.,
                & 0., 0.,50.,50., 0., 0., 0., 0., 0.,50.,50., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0.,50.,50.,50.,45.,25.,35.,45.,25.,25., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0.,40.,45.,50., 0.,40., 0., 0., 0.,10*0.,
                & 0.,50.,45.,35.,20.,15.,20.,25., 0., 0., 0.,50., 0., 0., 0.,10*0.,
                &50.,50.,50.,50., 0., 0.,30., 0., 0., 0., 0.,45., 0.,50.,50.,10*0.,
                & 0.,50.,50.,45.,45.,40.,35.,25.,35.,40.,45.,50.,50.,50., 0.,10*0.,
                & 0., 0., 0., 0.,45.,40., 0.,25.,40.,45., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0.,40.,30.,40.,35., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,40.,45.,35.,45., 0.,40., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,45.,45., 0.,50., 0.,40.,40.,45., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,45., 0., 0.,50., 0., 0.,40.,40.,45., 0., 0.,10*0.,
                & 0., 0., 0.,45.,45., 0., 0.,50., 0., 0., 0.,45.,45.,45., 0.,10*0.,
                  &95*0./
          C
0007               DATA FSLOW8/
                  &130*0.,
                  & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,50., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,50., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,50., 0., 0., 0., 0.,10*0.,
                  & 0., 0.,50.,50., 0., 0., 0., 0., 0.,50.,50., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0.,50.,50.,50.,45.,25.,35.,45.,25.,25., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0., 0., 0., 0.,40.,45.,50., 0.,40., 0., 0., 0.,10*0.,
                  & 0.,50.,45.,35.,20.,15.,20.,25., 0., 0., 0.,50., 0., 0., 0.,10*0.,
                  &50.,50.,50.,50., 0., 0.,30., 0., 0., 0., 0.,45., 0.,50.,50.,10*0.,
                  & 0.,50.,50.,45.,45.,40.,35.,25.,35.,40.,45.,50.,50.,50., 0.,10*0.,
                  & 0., 0., 0., 0.,45.,40., 0.,25.,40.,45., 0., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0., 0., 0.,40.,30.,40.,35., 0., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0.,40.,45.,35.,45., 0.,40., 0., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0.,45.,45., 0.,50., 0.,40.,40.,45., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0.,45., 0., 0.,50., 0., 0.,40.,40.,45., 0., 0.,10*0.,
                  & 0., 0., 0.,45.,45., 0., 0.,50., 0., 0., 0.,45.,45.,45., 0.,10*0.,
                  &95*0./
          C
0008               DATA FSLOW9/
                  &130*0.,
                  & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                  & 0., 0.,55.,55., 0., 0., 0., 0., 0.,55.,55., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0.,55.,55.,55.,50.,30.,40.,50.,30.,30., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0., 0., 0., 0.,45.,50.,55., 0.,45., 0., 0., 0.,10*0.,
                  & 0.,55.,50.,45.,30.,25.,30.,40., 0., 0., 0.,55., 0., 0., 0.,10*0.,
                  &55.,55.,55.,55., 0., 0.,40., 0., 0., 0., 0.,50., 0.,55.,55.,10*0.,
                  & 0.,55.,55.,50.,50.,45.,40.,35.,40.,45.,50.,55.,55.,55., 0.,10*0.,
                  & 0., 0., 0., 0.,50.,50., 0.,35.,45.,50., 0., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0., 0., 0.,45.,45.,45.,45., 0., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0.,45.,50.,40.,50., 0.,45., 0., 0., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0.,50.,50., 0.,55., 0.,45.,45.,50., 0., 0., 0.,10*0.,
                  & 0., 0., 0., 0.,50., 0., 0.,55., 0., 0.,45.,45.,50., 0., 0.,10*0.,
                  & 0., 0., 0.,50.,50., 0., 0.,55., 0., 0., 0.,50.,50.,50., 0.,10*0.,
                  &95*0./
          C
0009               END
```

```
0001             BLOCK DATA
           C
           C         BLOCK DATA PROGRAM NUMBER  THREE
           C
           C
0002             COMMON /DATFL3/ FFAST(25,25,4)
0003             DIMENSION FFAST6(625), FFAST7(625), FFAST8(625), FFAST9(625)
0004             EQUIVALENCE (FFAST6(1),FFAST(1,1,1)), (FFAST7(1),FFAST(1,1,2)),
                1             (FFAST8(1),FFAST(1,1,3)), (FFAST9(1),FFAST(1,1,4))
           C
0005             DATA FFAST6/
                &130*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                & 0., 0.,55.,55., 0., 0., 0., 0., 0.,55.,55., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0.,55.,55.,55.,50.,35.,45.,50.,35.,35., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0.,55.,55.,55., 0.,45., 0., 0., 0.,10*0.,
                & 0.,55.,55.,50.,45.,45.,45.,50., 0., 0., 0.,55., 0., 0., 0.,10*0.,
                &55.,55.,55.,55., 0., 0.,40., 0., 0., 0., 0.,50., 0.,55.,55.,10*0.,
                & 0.,55.,55.,50.,50.,50.,50.,45.,50.,50.,55.,55.,55.,55., 0.,10*0.,
                & 0., 0., 0., 0.,50.,50., 0.,50.,50.,50., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0.,55.,50.,55.,50., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,50.,55.,55.,55., 0.,55., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,55.,55., 0.,55., 0.,55.,55.,55., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,55., 0., 0.,55., 0., 0.,50.,50.,55., 0., 0.,10*0.,
                & 0., 0., 0.,55.,55., 0., 0.,55., 0., 0., 0.,50.,50.,50., 0.,10*0.,
                &95*0./
           C
0006             DATA FFAST7/
                &130*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                & 0., 0.,50.,50., 0., 0., 0., 0., 0.,50.,50., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0.,50.,50.,50.,50.,25.,35.,45.,25.,25., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0., 0.,50.,50.,50., 0.,40., 0., 0., 0.,10*0.,
                & 0.,50.,50.,40.,30.,30.,30.,40., 0., 0., 0.,50., 0., 0., 0.,10*0.,
                &50.,50.,50.,50., 0., 0.,35., 0., 0., 0., 0.,45., 0.,50.,50.,10*0.,
                & 0.,50.,50.,45.,45.,45.,45.,35.,40.,40.,50.,50.,50.,50., 0.,10*0.,
                & 0., 0., 0., 0.,50.,50., 0.,50.,50.,50., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0., 0., 0.,50.,45.,50.,45., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,40.,50.,50.,50., 0.,50., 0., 0., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,45.,50., 0.,50., 0.,50.,50.,50., 0., 0., 0.,10*0.,
                & 0., 0., 0., 0.,50., 0., 0.,50., 0., 0.,50.,50.,50., 0., 0.,10*0.,
                & 0., 0., 0.,50.,50., 0., 0.,50., 0., 0., 0.,45.,45.,45., 0.,10*0.,
                       &95*0./
               C
0007                    DATA FFAST8/
                       &130*0.,
                       & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                       & 0., 0.,50.,50., 0., 0., 0., 0., 0.,50.,50., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0.,50.,50.,50.,50.,25.,35.,45.,25.,25., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0., 0., 0., 0.,50.,50.,50., 0.,40., 0., 0., 0.,10*0.,
                       & 0.,50.,50.,40.,30.,30.,30.,40., 0., 0., 0.,50., 0., 0., 0.,10*0.,
                       &50.,50.,50.,50., 0., 0.,35., 0., 0., 0., 0.,45., 0.,50.,50.,10*0.,
                       & 0.,50.,50.,45.,45.,45.,45.,35.,40.,40.,50.,50.,50.,50., 0.,10*0.,
                       & 0., 0., 0., 0.,50.,50., 0.,50.,50.,50., 0., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0., 0., 0.,50.,45.,50.,45., 0., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0.,40.,50.,50.,50., 0.,50., 0., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0.,45.,50., 0.,50., 0.,50.,50.,50., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0.,50., 0., 0.,50., 0., 0.,50.,50.,50., 0., 0.,10*0.,
                       & 0., 0., 0.,50.,50., 0., 0.,50., 0., 0., 0.,45.,45.,45., 0.,10*0.,
                       &95*0./
               C
0008                    DATA FFAST9/
                       &130*0.,
                       & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,55., 0., 0., 0., 0.,10*0.,
                       & 0., 0.,55.,55., 0., 0., 0., 0., 0.,55.,55., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0.,55.,55.,55.,50.,30.,40.,50.,30.,30., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0., 0., 0., 0.,55.,55.,55., 0.,45., 0., 0., 0.,10*0.,
                       & 0.,55.,55.,50.,40.,40.,40.,50., 0., 0., 0.,55., 0., 0., 0.,10*0.,
                       &55.,55.,55.,55., 0., 0.,45., 0., 0., 0., 0.,50., 0.,55.,55.,10*0.,
                       & 0.,55.,55.,50.,50.,50.,50.,45.,50.,50.,55.,55.,55.,55., 0.,10*0.,
                       & 0., 0., 0., 0.,50.,50., 0.,45.,50.,50., 0., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0., 0., 0.,55.,50.,55.,50., 0., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0.,45.,55.,55.,55., 0.,55., 0., 0., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0.,50.,55., 0.,55., 0.,55.,55.,55., 0., 0., 0.,10*0.,
                       & 0., 0., 0., 0.,55., 0., 0.,55., 0., 0.,50.,50.,55., 0., 0.,10*0.,
                       & 0., 0., 0.,50.,50., 0., 0.,55., 0., 0., 0.,50.,50.,50., 0.,10*0.,
                       &95*0./
               C
0009                    END
```

```
0001                 BLOCK DATA
               C
               C          BLOCK DATA PROGRAM NUMBER  FOUR
               C
               C
0002                 COMMON /DATFL4/ FRATIO(25,25,4)
0003                 DIMENSION FRAT6(625), FRAT7(625), FRAT8(625), FRAT9(625)
0004                 EQUIVALENCE (FRAT6(1),FRATIO(1,1,1)), (FRAT7(1),FRATIO(1,1,2)),
                    1            (FRAT8(1),FRATIO(1,1,3)), (FRAT9(1),FRATIO(1,1,4))
               C
0005                 DATA FRAT6/
                    &130*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.8,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.8,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.8,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,2.2,2.2,0.0,0.0,0.0,0.0,0.0,1.8,1.8,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,2.2,2.2,2.2,1.8,1.2,1.8,2.0,1.2,1.2,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,0.0,2.2,2.0,1.8,0.0,1.2,0.0,0.0,0.0,10*0.,
                    &0.0,1.8,2.2,2.2,1.8,1.8,1.8,2.2,0.0,0.0,0.0,1.8,0.0,0.0,0.0,10*0.,
                    &2.2,2.2,1.8,1.8,0.0,0.0,1.5,0.0,0.0,0.0,0.0,2.2,0.0,2.2,2.2,10*0.,
                    &0.0,1.6,2.0,2.2,2.7,3.5,3.5,1.2,1.8,1.8,2.2,2.2,2.3,2.3,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,1.8,1.8,0.0,2.2,1.2,1.2,0.0,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,3.5,3.5,3.5,3.5,0.0,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,3.5,3.5,3.5,2.2,0.0,2.2,0.0,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,3.5,3.5,0.0,2.2,0.0,2.2,2.2,2.2,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,3.5,0.0,0.0,2.2,0.0,0.0,2.2,2.2,2.2,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,3.5,1.8,0.0,0.0,2.2,0.0,0.0,0.0,2.2,2.2,2.2,0.0,10*0.,
                    &95*0./
               C
0006                 DATA FRAT7/
                    &130*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.5,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.5,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.5,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,1.9,1.9,0.0,0.0,0.0,0.0,0.0,1.5,1.5,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,1.9,1.9,1.9,1.5,1.0,1.5,1.7,1.0,1.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.9,1.7,1.5,0.0,1.0,0.0,0.0,0.0,10*0.,
                    &0.0,1.5,1.9,1.9,1.5,1.5,1.5,1.9,0.0,0.0,0.0,1.5,0.0,0.0,0.0,10*0.,
                    &1.9,1.9,1.5,1.5,0.0,0.0,1.2,0.0,0.0,0.0,0.0,1.9,0.0,1.9,1.9,10*0.,
                    &0.0,1.3,1.7,1.9,2.3,3.0,3.0,1.0,1.5,1.5,1.9,1.9,2.0,2.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,1.5,1.5,0.0,1.9,1.0,1.0,0.0,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,0.0,0.0,3.0,3.0,3.0,3.0,0.0,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,3.0,3.0,3.0,1.9,0.0,1.9,0.0,0.0,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,3.0,3.0,0.0,1.9,0.0,1.9,1.9,1.9,0.0,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,0.0,3.0,0.0,0.0,1.9,0.0,0.0,1.9,1.9,1.9,0.0,0.0,10*0.,
                    &0.0,0.0,0.0,3.0,1.5,0.0,0.0,1.9,0.0,0.0,0.0,1.9,1.9,1.9,0.0,10*0.,
                   &95*0./
              C
0007                DATA FRAT8/
                   &130*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.5,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.5,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.5,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,1.9,1.9,0.0,0.0,0.0,0.0,0.0,1.5,1.5,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,1.9,1.9,1.9,1.5,1.0,1.5,1.7,1.0,1.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.9,1.7,1.5,0.0,1.0,0.0,0.0,0.0,10*0.,
                   &0.0,1.5,1.9,1.9,1.5,1.5,1.5,1.9,0.0,0.0,0.0,1.5,0.0,0.0,0.0,10*0.,
                   &1.9,1.9,1.5,1.5,0.0,0.0,1.2,0.0,0.0,0.0,0.0,1.9,0.0,1.9,1.9,10*0.,
                   &0.0,1.3,1.7,1.9,2.3,3.0,3.0,1.0,1.5,1.5,1.9,1.9,2.0,2.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,1.5,1.5,0.0,1.9,1.0,1.0,0.0,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,3.0,3.0,3.0,3.0,0.0,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,3.0,3.0,3.0,1.9,0.0,1.9,0.0,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,3.0,3.0,0.0,1.9,0.0,1.9,1.9,1.9,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,3.0,0.0,0.0,1.9,0.0,0.0,1.9,1.9,1.9,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,3.0,1.5,0.0,0.0,1.9,0.0,0.0,0.0,1.9,1.9,1.9,0.0,10*0.,
                   &95*0./
              C
0008                DATA FRAT9/
                   &130*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.3,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.3,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.3,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,1.5,1.5,0.0,0.0,0.0,0.0,0.0,1.3,1.3,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,1.5,1.5,1.5,1.3,1.0,1.3,1.3,1.0,1.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,0.0,1.5,1.3,1.3,0.0,1.0,0.0,0.0,0.0,10*0.,
                   &0.0,1.3,1.5,1.5,1.3,1.3,1.3,1.5,0.0,0.0,0.0,1.3,0.0,0.0,0.0,10*0.,
                   &1.5,1.5,1.3,1.3,0.0,0.0,1.1,0.0,0.0,0.0,0.0,1.5,0.0,1.5,1.5,10*0.,
                   &0.0,1.2,1.3,1.5,2.0,2.5,2.5,1.0,1.3,1.3,1.5,1.5,1.7,1.7,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,1.3,1.3,0.0,1.5,1.0,1.0,0.0,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,0.0,0.0,2.5,2.5,2.5,2.5,0.0,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,2.5,2.5,2.5,1.5,0.0,1.5,0.0,0.0,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,2.5,2.5,0.0,1.5,0.0,1.5,1.5,1.5,0.0,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,0.0,2.5,0.0,0.0,1.5,0.0,0.0,1.5,1.5,1.5,0.0,0.0,10*0.,
                   &0.0,0.0,0.0,2.5,1.3,0.0,0.0,1.5,0.0,0.0,0.0,1.5,1.5,1.5,0.0,10*0.,
                   &95*0./
              C
0009                END
```

```
            BLOCK DATA
C
C               BLOCK DATA PROGRAM NUMBER  FIVE
C
            COMMON /COLDST/ NBETA, TCS(20), CSF(60)
            COMMON /GRID/ X1, X2, Y1, Y2, NX, NY, DELX, DELY, DELT
            COMMON /TABLES/ THOUR(24), TZ(8), YFR(8)
            COMMON /SPDFCT/ A(3), B(3), C(3), VBAR
C
            DATA NBETA/20/, TCS/360., 365., 370., 375., 380., 385., 390.,
           1  395., 400., 410., 420., 425., 430., 435., 440., 500., 520.,
           2  535., 550., 560./, CSF/20*1.0, 1.0, 1.057, 1.087, 1.074, 1.054,
           3  1.038, 1.029, 1.023, 1.019, 1.014, 1.011, 1.007, 1.002, 0.998,
           4  0.996, 0.994, 0.992, 0.989, 0.998, 1.0,   1.0,   1.186, 1.287,
           5  1.243, 1.179, 1.125, 1.094, 1.075, 1.063, 1.047, 1.038, 1.025,
           6  1.007, 0.995, 0.988, 0.979, 0.972, 0.965, 0.993, 1.0 /
            DATA X1,X2,Y1,Y2/0.,50.,0.,50./, NX,NY/25,25/, DELX,DELY/2.,2./
            DATA THOUR/0.,60.,120.,180.,240.,300.,360.,420.,480.,540.,600.,
           1  660.,720.,780.,840.,900.,960.,1020.,1080.,1140.,1200.,1260.,
           2  1320.,1380./
            DATA TZ/0., 360., 540., 690., 810., 990., 1110., 1260./
            DATA YFR/0.90, 0.85, 0.25, 0.30, 0.20, 0.50, 0.15, 0.20/
            DATA B/0.,-0.662,-0.842/,C/0.0295,0.,0./,VBAR/44./
C
            END
```

APPENDIX B

INPUT FOR DIFKIN RUN

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS
 IS TRAJECTORY INPUT EXTERNALLY        NO
 ARE FLUXES INPUT EXTERNALLY           NO
 DO WE COMPUTE SPECIES CONCENTRATIONS  YES       NO
 PRINT STATION COORDS, WIND DATA       YES       YES
730813 1CWELSCENTENNIAL WELL36PT212121 33336332727 3 621242736 33636363318212124
730813 1CWELSCENTENNIAL WELLMPH  3 3 2 / 5 6 3 2 2 3 4 3 3 3 4 5 5 6 8 4 3 4 4 4
730813 2DWW  DENVER SEWER   36PT2929313131313431313 6 6 4 2363436343431 236181618
730813 2DWW  DENVER SEWER   MPH  7121513 7 3 1 3 4 3 5 4 5 3 4 4 7 7 9 6 2 7 8 8
730813 3BRIN BRIGHTON       36PT3036 33636 3 6 912151518181818 33633 6 918212421
730813 3BRIN BRIGHTON       MPH  3 5 911 7 4 5 5 5 7 5 7 7 5 5 5 5 6 8 3 3 4 6 7
999999
WIND SPEED MULTIPLIER                  1.0
DO WE WANT EXTRA TRAJECTORY OUTPUT     NO
START DATE AND LOCAL TIME(24HR CLOCK)  730813    1400
IS LOCAL TIME STANDARD OR DAYLIGHT     STANDARD
START LOCATION (STATION ID OR COORDS)            20.00     32.00
TRAJECTORY DURATION, HOURS             4.0
TRAJECTORY SEGMENT LENGTH, HOURS       1.0
STARTING AZIMUTH AND VELOCITY %OPTIONAL<
DIRECTION FLAG (POS=FRWRD, NEG=BKWRD)  -1
WEIGHTING FLAG %01#1/R, 02#1/R**2<     01
NUMBER OF CLOSE STATIONS TO USE        03
GRID BOUNDARIES %ST.MI.<      0.       50.       8.00      41.33333
HOT-START EMISSION FACTORS, GM/MI      2.34      7.7       95.4
COLD-START EMISSION FACTORS, GM/MI     2.34      7.7       95.4
1969/1969 GROWTH FACTORS  AUTO, STAT   1.0       1.0
FREEWAY VEHICLE ADJUST. FACTORS        1.0       1.0       1.0
SURFACE ST. VEHICLE ADJUST.FACTORS     1.0       1.0       1.0
POWER PLANT ADJUST. FACTORS            1.0
OIL REFINERY ADJUST. FACTORS           1.0       1.0
AREA STATIONARY ADJUST. FACTORS        1.0       1.0
  INITIAL TIME STEP                    .01
  UPPER LIMIT FRACTIONAL CHANGE        .03
  LOWER LIMIT FRACTIONAL CHANGE        0.01
  PRINT INTERVAL                       30.
  UPPER LIMIT ON DELT                  0.5
  LOWER LIMIT ON DELT                  0.002
  VERTICAL MESH INTERVAL %METERS<      115.
  TIME INTERVAL FOR UPDATING K1        10.
  DO WE WANT A FIXED STEP SIZE         NO
  SHALL WE OUTPUT THE TIME STEPS       NO
  SHALL WE OUTPUT THE EXECUTION TIMES  YES
  SHALL WE OUTPUT EVERY CYCLE          NO
  DO WE WANT PUNCHED OUTPUT            NO
  IS K1 VARIABLE                       YES
  IS INVERSION HEIGHT VARIABLE         YES
  DO WE HAVE ONLY AN INERT SPECIES     NO
  NUMBER OF INTEGRATION STEPS               25000
  NUMBER OF REACTIONS                          16
  NUMBER OF SPECIES                            10
  NUMBER OF SPECIES IN STEADY STATE             4
  NUMBER OF TRACER SPECIES %0 OR 1<             1
  HOW MANY SPECIES HAVE A FLUX                  3
  NUMBER OF VERTICAL STATIONS                   5
  SPECIES NAME AND MOLE WEIGHT         NO        30.01
```

```
                                        HC        72.20
                                        NO2       46.01
                                        OZON      48.
                                        HNO2      47.00
                                        NO3       62.
                                        N2O5      108.
                                        OH        17.
                                        RO2       68.1
                                        CO        28.00
POSITION OF FIRST SPECIES WITH FLUX              1
POSITION OF SECOND SPECIES WITH FLUX             2
POSITION OF THIRD SPECIES WITH FLUX             10
NO   PPHM           1.00      1.00      1.00      1.00      1.00
HC   PPHM           1.00      1.00      1.00      1.00      1.00
NO2  PPHM           1.00      1.00      1.00      1.00      1.00
O3   PPHM           1.558     1.558     1.558     1.558     1.558
HNO2 PPHM           1.00      1.00      1.00      1.00      1.0
NO3 PPHM - COMPUTED                                                    BY CODE
N2O5 PPHM- COMPUTED                                                    BY CODE
OH   PPHM- COMPUTED                                                    BY CODE
RO2  PPHM- COMPUTED                                                    BY CODE
CO   PPHM           200.0     200.0     200.0     200.0     200.0
  RATE CONSTANTS -  REACTION NO.  1 %K1<          OBTAINED FROM -UPRATE-
                    REACTION NO.  2     .267
                    REACTION NO.  3       1.000E-6
                    REACTION NO.  4     100.
                    REACTION NO.  5         1.0E+3
                    REACTION NO.  6     2.0
                    REACTION NO.  7     15.
                    REACTION NO.  8     30.
                    REACTION NO.  9        4.00E-5
                    REACTION NO. 10               OBTAINED FROM -UPRATE-
                    REACTION NO. 11         5.0E-5
                    REACTION NO. 12     45.
                    REACTION NO. 13     14.
                    REACTION NO. 14     60.5
                    REACTION NO. 15         0.0
                    REACTION NO. 16     .001
PHOTON & NO2 # NO  & O3
NO     & O3  # NO2 & O2
O      & HC  # 8RO2
OH     & HC  # 8RO2
RO2    & NO  # NO2 & .125*OH
RO2    & NO2 # PAN
OH     & NO  # HNO2
OH     & NO2 # HNO3
O3     & HC  # RO2
PHOTON & HONO# OH & NO
NO2    & O3  # NO3 & O2
NO3    & NO2 # N2O5
N2O5         # NO3 & NO2
N2O5   & H2O # 2HNO3
NO & NO2 & H2O # 2HNO2
NO2 & PARTICLES # PRODUCTS
0.        1.                  BEGIN NO            STOICHIOMETRIC COEFFICIENTS
1.        0
```

```
0         0
0         0
1.        0
0         0
1.        0
0         0
0         0
0         1.
0.        0.
0.        0.
0.        0.
0.        0.
1.        0.
0.        0.                    END NO
0.        0.                    BEGIN HYDROCARBON
0         0
1.        0.
1.        0
0         0
0         0
0         0
0         0
1.        0
0         0
0         0
0.        0.
0.        0.
0.        0.
0.        0.
0.        0.                    END HYDROCARBON
1.        0.                    BEGIN NO2
0         1.
0         0
0         0
0         1.
1.        0
0         0
1.        0
0         0
0         0
1.        0
1.        0.
0.        1.
0         0
1.        0.
1.        0.                    END NO2
0.        1.                    BEGIN OZONE
1.        0
0         0
0         0
0         0
0         0
0         0
0         0
1.        0
0         0
```

```
1.          0.
0.          0.
0.          0.
0.          0.
0.          0.
0.          0.                    END OZONE
0.          0.                    BEGIN HNO2
0           0
0           0
0           0
0           0
0           0
0           1.
0           0
0           0
1.          0
0           0
0.          0.
0.          0.
0.          0.
0.          2.
0.          0.                    END HNO2
0.          0.                    BEGIN NO3
0           0
0           0
0           0
0           0
0           0
0           0
0           0
0           0
0           0
0           1.
1.          0
0.          1.
0.          0.
0.          0.
0.          0.                    END NO3
0.          0.                    BEGIN N2O5
0.          0.
0.          0.
0.          0.
0.          0.
0.          0.
0.          0.
0.          0.
0.          0.
0.          0.
0.          0.
0.          1.
1.          0.
1.          0.
0.          0.
0.          0.                    END N2O5
0.          0.                    BEGIN OH
0           0
```

```
0         0
1.        0
0.        0.125
0         0
1.        0
1.        0
0         0
0         1.
0         0
0.        0.
0.        0.
0.        0.
0.        0.
0.        0.                    END OH
0.        0.                    BEGIN RO2
0         0
0.        8.
0.        8.
1.        0
1.        0
0         0
0         0
0.        1.
0         0
0         0
0.        0.
0.        0.
0.        0.
0.        0.
0.        0.                    END RO2                 END STOICHIOMETRY
  1000    K1              0.41609E 00
  1010                    0.42082E 00
  1020                    0.42536E 00
  1030                    0.42967E 00
  1040                    0.43373E 00
  1050                    0.43750E 00
  1100                    0.44094E 00
  1110                    0.44401E 00
  1120                    0.44665E 00
  1130                    0.44883E 00
  1140                    0.45051E 00
  1150                    0.45165E 00
  1200                    0.45222E 00
  1210                    0.45222E 00
  1220                    0.45164E 00
  1230                    0.45050E 00
  1240                    0.44882E 00
  1250                    0.44664E 00
  1300                    0.44399E 00
  1310                    0.44093E 00
  1320                    0.43749E 00
  1330                    0.43371E 00
  1340                    0.42965E 00
  1350                    0.42534E 00
  1400                    0.42080E 00
  1410                    0.41607E 00
  1420                  0.41117E 00
  1430                  0.40553E 00
  1440                  0.39462E 00
  1450                  0.38349E 00
  1500                  0.37217E 00
  1510                  0.36067E 00
  1520                  0.34904E 00
  1530                  0.33728E 00
  1540                  0.32542E 00
  1550                  0.31348E 00
  1600                  0.30147E 00
  1610                  0.28940E 00
  1620                  0.27572E 00
  1630                  0.25655E 00
  1640                  0.23734E 00
  1650                  0.21812E 00
  1700                  0.19890E 00
 LAST CARD K1           -10.
 DIFF. UPDATE       0.          865.        60.         150.        150.
                    150.        150.        150.
 DIFF. UPDATE       100.        865.        60.         600.        600.
                    600.        600.        600.
 DIFF. UPDATE       500.        865.        60.         3000.       3000.
                    3000.       3000.       3000.
 LAST CARD          -10.
 2ND LAST CARD
 END
```

APPENDIX C

OUTPUT FROM DIFKIN RUN

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS                CP TIME =    0.000DATE        QTO-

        STATIONS AND COORDINATES

        1CWELS       25.00      21.00
        2DWW         27.00      33.00
        3BRIN        35.00      45.00
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS            CP TIME =    0.00DATE       QTO-

                                                     WIND DATA

730813 1CWELS              36.PT21.21.21. 3.33.36.33.27.27. 3. 6.21.24.27.36. 3.36.36.36.33.18.21.21.24.
                                3. 3. 2. 7. 5. 6. 3. 2. 2. 3. 4. 3. 3. 3. 4. 5. 5. 6. 8. 4. 3. 4. 4. 4.
730813 2DWW                36.PT29.29.31.31.31.31.34.31.31.36. 6. 4. 2.36.34.36.34.34.31. 2.36.18.16.18.
                                7.12.15.13. 7. 3. 1. 3. 4. 3. 5. 4. 5. 3. 4. 4. 7. 7. 9. 6. 2. 7. 8. 8.
730813 3BRIN               36.PT30.36. 3.36.36. 3. 6. 9.12.15.15.18.18.18.18. 3.36.33. 6. 9.18.21.24.21.
                                3. 5. 9.11. 7. 4. 5. 5. 5. 7. 5. 7. 7. 5. 5. 5. 5. 6. 8. 3. 3. 4. 6. 7.
```

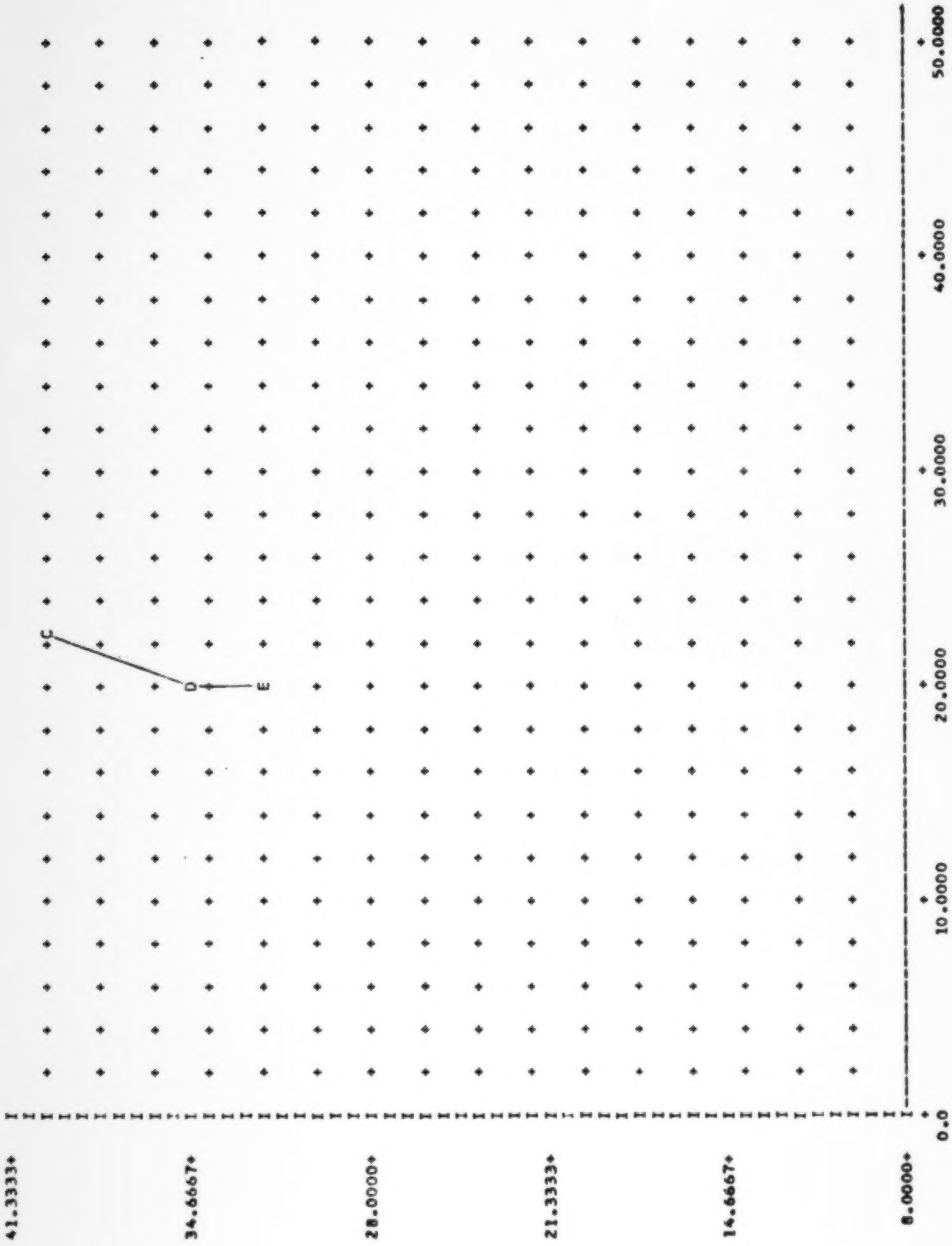
```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS               CP TIME =    0.000DATE       QTO-

AIR TRAJECTORY CALCULATION DATA

   START DATE AND LOCAL TIME AT INITIAL POINT              730813    1400 HRS (STANDARD TIME)
   LOCATION OF INITIAL POINT                                20.00     32.00   (NOT AT A MEASUREMENT STATION)
   PRESCRIBED STARTING AZIMUTH AND VELOCITY (OPTIONAL)
   DIRECTION OF TRAJECTORY DEVELOPMENT                     BACKWARD
   DESIRED TRAJECTORY DURATION                               4.0 HRS
   TRAJECTORY SEGMENT LENGTH                                 1.0 HRS
   WIND MEASUREMENT INTERPOLATION SCHEME                   3  CLOSEST STATIONS WITH  1/R  WEIGHTING


GRID REFERENCE DATA
                         LATITUDE      LONGITUDE          X(ST MI)     Y(ST MI)      I      J
      CENTER             39/44/58.0    104/59/22.0         25.000       25.000      13     13
      ORIGIN             39/23/14.4    105/27/37.2          0.0          0.0         1      1
      START POINT        40/ 6/ 2.8    105/ 0/13.4         24.240       49.262      13     25
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS             CP TIME =   0.00DATE      QTO-
TRAJECTORY DATA
  SYMBOL  T(MIN)     I     J      X(MI)      Y(MI)      V(MPH)    THETA
     A      0.0     13    25      24.24      49.26       5.00     292.50
     B     60.00    14    23      26.15      44.64       5.71     232.82
     C    120.00    12    21      22.70      40.10       5.77     242.04
     D    180.00    10    18      20.00      35.00       3.00     270.00
     E    240.00    10    16      20.00      32.00       3.00     270.00
```


41.3333+
34.6667+
28.0000+
21.3333+
14.6667+
8.0000+
0.0
10.0000
20.0000
30.0000
40.0000
50.0000
C
D
E

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS            CP TIME =    0.00DATE       QTO-
   TC(MIN)     XC(MI)     YC(MI)     IC     JC
    16.39      24.76      48.00      13     24
    42.36      25.59      46.00      13     23
    55.20      26.00      45.01      14     23
    62.66      26.00      44.44      13     23
    68.48      25.67      44.00      13     22
    94.87      24.15      42.00      13     21
    97.46      24.00      41.80      12     21
   121.13      22.65      40.00      12     20
   135.63      22.00      38.77      11     20
   144.68      21.59      38.00      11     19
   168.23      20.53      36.00      11     18
   180.00      20.00      35.00      10     18
   200.00      20.00      34.00      10     17
   240.00      20.00      32.00      10     16
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS            CP TIME =    0.000DATE       QTO-

                                   SOURCE FLUX CONTRIBUTIONS (KG/HR)

LOCAL                              NITRIC OXIDE          REACTIVE HYDROCARBONS        CARBON MONOXIDE
 TIME        I     J           VEHICLE   STATIONARY       VEHICLE   STATIONARY       VEHICLE   STATIONARY

1000.       13    25              0.0         0.0             0.0         0.0            0.0         0.0
1016.       13    24              0.0         0.0             0.0         0.0            0.0         0.0
1042.       13    23              0.0         0.0             0.0         0.0            0.0         0.0
1055.       14    23              0.0         0.0             0.0         0.0            0.0         0.0
1100.       14    23              0.0         0.0             0.0         0.0            0.0         0.0
1103.       13    23              0.0         0.0             0.0         0.0            0.0         0.0
1108.       13    22              0.0         0.0             0.0         0.0            0.0         0.0
1130.       13    22              0.0         0.0             0.0         0.0            0.0         0.0
1135.       13    21              3.52        0.0             5.60        0.0           85.13        0.0
1137.       12    21              0.13        0.0             0.44        9.15           7.82        0.0
1200.       12    21              0.13        0.0             0.47        9.15           8.20        0.0
1201.       12    20              1.18        0.0             4.20        0.0           73.84        0.0
1216.       11    20              1.71       62.61            6.06      175.29         106.66        0.0
1225.       11    19              6.02        2.61           11.12       79.55         175.89        0.0
1249.       11    18              6.78        0.0            15.16        0.0          249.52        0.0
1260.       10    18              0.88        5.87            1.79       54.21          28.92        0.0
1300.       10    18              0.86        5.87            1.75       54.21          28.25        0.0
1320.       10    17              1.92        1.96            6.83        2.11         120.20        0.0
1330.       10    17              1.92        1.96            6.83        2.11         120.20        0.0
1360.       10    16              8.00       42.39           26.93      143.61         471.02        0.0
1400.       10    16              8.95       42.39           30.13      143.61         527.09        0.0
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS                    CP TIME =    0.000ATE       QTO-

    TOTAL FLUXES IN UNITS USED BY CODE (M/MIN)

    TIME         NITRIC OXIDE     REACTIVE HYDROCARBONS      CARBON MONOXIDE
     0.0            0.0               0.0                       0.0
    16.4            0.0               0.0                       0.0
    42.4            0.0               0.0                       0.0
    55.2            0.0               0.0                       0.0
    60.0            0.0               0.0                       0.0
    62.7            0.0               0.0                       0.0
    68.5            0.0               0.0                       0.0
    90.0            0.0               0.0                       0.0
    94.9            0.5717E-08        0.9092E-08                0.1383E-06
    97.5            0.2034E-09        0.1559E-07                0.1271E-07
   120.0            0.2133E-09        0.1563E-07                0.1333E-07
   121.1            0.1919E-08        0.6818E-08                0.1200E-06
   135.6            0.1045E-06        0.2947E-06                0.1733E-06
   144.7            0.1402E-07        0.1473E-06                0.2858E-06
   168.2            0.1102E-07        0.2463E-07                0.4055E-06
   180.0            0.1097E-07        0.9100E-07                0.4699E-07
   180.0            0.1094E-07        0.9093E-07                0.4590E-07
   200.0            0.6304E-08        0.1453E-07                0.1953E-06
   210.0            0.6304E-08        0.1453E-07                0.1953E-06
   240.0            0.8188E-07        0.2771E-06                0.7654E-06
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS            CP TIME =    0.00DATE       QTO-  PAGE    8
INPUT DATA FOR VERTICAL DIFFUSION PROBLEM WITH PHOTOCHEMISTRY
 INITIAL TIME IS 0.0         MINUTES
 FINAL TIME IS 0.24000E 03 MINUTES
 TIME STEP SIZE IS 0.10000E-01 MINUTES
 VERTICAL MESH INCREMENT IS 0.11500E 03 METERS
 NUMBER OF REACTIONS IS 16
 NUMBER OF SPECIES IS 10
 NUMBER OF SPECIES IN STEADY STATE IS   4
 NUMBER OF TRACER SPECIES IS   1   (CANNOT EXCEED 1)
 NUMBER OF VERTICAL MESH POINTS IS  5 INCLUDING THE GROUND AND THE EDGE
 STEP SIZE CONTROLS
        UPPER LIMIT FRACTIONAL CHANGE IS 0.30000E-01
        LOWER LIMIT FRACTIONAL CHANGE IS 0.10000E-01

              NO        HC        NO2       OZON      HNO2      NO3       N2O5      OH         RATE CONSTANT
              RO2
 REACTION                         - - - R E A C T A N T   S T O I C H I O M E T R Y - - -      (PPHM/MIN)
    1         0.0       0.0       1.0       0.0       0.0       0.0       0.0       0.0        0.41609
             0.0
    2         1.0       0.0       0.0       1.0       0.0       0.0       0.0       0.0        0.26700
             0.0
    3         0.0       1.0       0.0       0.0       0.0       0.0       0.0       0.0        0.10000E-05
             0.0
    4         0.0       1.0       0.0       0.0       0.0       0.0       0.0       1.0         100.00
             0.0
    5         1.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0         1000.0
             1.0
    6         0.0       0.0       1.0       0.0       0.0       0.0       0.0       0.0         2.0000
             1.0
    7         1.0       0.0       0.0       0.0       0.0       0.0       0.0       1.0         15.000
             0.0
    8         0.0       0.0       1.0       0.0       0.0       0.0       0.0       1.0         30.000
             0.0
    9         0.0       1.0       0.0       1.0       0.0       0.0       0.0       0.0        0.40000E-04
             0.0
```

```
10       0.0      0.0      0.0      0.0      1.0      0.0      0.0      0.0         0.15584E-02
        0.0
11       0.0      0.0      1.0      1.0      0.0      0.0      0.0      0.0         0.50000E-04
        0.0
12       0.0      0.0      1.0      0.0      0.0      1.0      0.0      0.0          45.000
        0.0
13       0.0      0.0      0.0      0.0      0.0      0.0      1.0      0.0          14.000
        0.0
14       0.0      0.0      0.0      0.0      0.0      0.0      1.0      0.0          60.500
        0.0
15       1.0      0.0      1.0      0.0      0.0      0.0      0.0      0.0         0.0
        0.0
16       0.0      0.0      1.0      0.0      0.0      0.0      0.0      0.0         0.10000E-02
        0.0
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS          CP TIME =    0.00DATE

REACTION                          - - - P R O D U C T   S T O I C H I O M E T R Y - - -
    1           1.00      0.0       0.0       1.00      0.0       0.0       0.0       0.0
               0.0
    2           0.0       0.0       1.00      0.0       0.0       0.0       0.0       0.0
               0.0
    3           0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
               8.00
    4           0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
               8.00
    5           0.0       0.0       1.00      0.0       0.0       0.0       0.0       0.13
               0.0
    6           0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
               0.0
    7           0.0       0.0       0.0       0.0       1.00      0.0       0.0       0.0
               0.0
    8           0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
               0.0
    9           0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
               1.00
   10           1.00      0.0       0.0       0.0       0.0       0.0       0.0       1.00
               0.0
   11           0.0       0.0       0.0       0.0       0.0       1.00      0.0       0.0
               0.0
   12           0.0       0.0       0.0       0.0       0.0       0.0       1.00      0.0
               0.0
   13           0.0       0.0       1.00      0.0       0.0       1.00      0.0       0.0
               0.0
   14           0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
               0.0
   15           0.0       0.0       0.0       0.0       2.00      0.0       0.0       0.0
               0.0
   16           0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
               0.0
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS                CP TIME =    0.000ATE

                      R E A C T I O N S
            1.     PHOTON & NO2 # NO  & O3
            2.     NO     & O3  # NO2 & O2
            3.     O      & HC  # 8RO2
            4.     OH     & HC  # 8RO2
            5.     RO2    & NO  # NO2 & .125*OH
            6.     RO2    & NO2 # PAN
            7.     OH     & NO  # HNO2
            8.     OH     & NO2 # HNO3
            9.     O3     & HC  # RO2
           10.     PHOTON & HONO# OH & NO
           11.     NO2    & O3  # NO3 & O2
           12.     NO3    & NO2 # N2O5
           13.     N2O5         # NO3 & NO2
           14.     N2O5   & H2O # 2HNO3
           15.     NO & NO2 & H2O # 2HNO2
           16.     NO2 & PARTICLES # PRODUCTS
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS                CP TIME =    0.000ATE


                   - - - - - - - - - - -

  SPECIES          FLUXES            MOLE WT
          NO       0.0               0.30010E 02
          HC       0.0               0.72200E 02
          NO2      0.0               0.46010E 02
          OZON     0.0               0.48000E 02
          HNO2     0.0               0.47000E 02
          NO3      0.0               0.62000E 02
          N2O5     0.0               0.10800E 03
          OH       0.0               0.17000E 02
          RO2      0.0               0.68100E 02
          CO       0.0               0.28000E 02
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS            CP TIME =    0.000ATE
          INITIAL DIFFUSION COEFFICIENTS
         VALUES SHOWN ARE FOR POINTS HALFWAY BETWEEN STATIONS

         STATION          HEIGHT (METERS)          DIFFUSIVITY
            1                     0.0               59.999954
                                                    149.99997
            2                  115.00
                                                    149.99997
            3                  230.00
                                                    149.99997
            4                  345.00
                                                    149.99997
            5                  460.00               149.99997
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS          CP TIME =   0.00DATE      QTO-



                    INITIAL PROFILES OF CONCENTRATIONS-PPHM


HEIGHT-M.      NO             HC             NO2            OZON           HNO2           NO3            N2O5           OH
                  RO2            CO

  0.0      0.10000E 01    0.10000E 01    0.10000E 01    0.15580E 01    0.10000E 01    0.21317E-05    0.12876E-05    0.34659E-04
           0.27737E-04    0.20000E 03

115.00     0.10000E 01    0.10000E 01    0.10000E 01    0.15580E 01    0.10000E 01    0.21317E-05    0.12876E-05    0.34659E-04
           0.27737E-04    0.20000E 03

230.00     0.10000E 01    0.10000E 01    0.10000E 01    0.15580E 01    0.10000E 01    0.21317E-05    0.12876E-05    0.34659E-04
           0.27737E-04    0.20000E 03

345.00     0.10000E 01    0.10000E 01    0.10000E 01    0.15580E 01    0.10000E 01    0.21317E-05    0.12876E-05    0.34659E-04
           0.27737E-04    0.20000E 03

460.00     0.10000E 01    0.10000E 01    0.10000E 01    0.15580E 01    0.10000E 01    0.21317E-05    0.12876E-05    0.34659E-04
           0.27737E-04    0.20000E 03
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS            CP TIME =    0.000DATE      QTO-  PAGE    14



                          CONCENTRATION PROFILES-PARTS PER HUNDRED MILLION

                                       TIME= 0.30000E 02 MINUTES

         GROUND DIFFUSIVITY =  59.999954                  K1 = 0.42535996
     NO   FLUX =     0.0
     HC   FLUX =     0.0
     CO   FLUX =     0.0

    HEIGHT-M.   NO              HC              NO2             OZON            HNO2            NO3             N2O5            OH
                  RO2             CO

       0.0      0.84734E 00     0.90167E 00     0.11270E 01     0.20416E 01     0.96735E 00     0.27934E-05     0.19015E-05     0.33164E-04
                0.28248E-04     0.20000E 03

     115.00     0.84734E 00     0.90167E 00     0.11270E 01     0.20416E 01     0.96735E 00     0.27934E-05     0.19015E-05     0.33164E-04
                0.28248E-04     0.20000E 03

     230.00     0.84734E 00     0.90167E 00     0.11270E 01     0.20416E 01     0.96735E 00     0.27934E-05     0.19015E-05     0.33164E-04
                0.28248E-04     0.20000E 03

     345.00     0.84734E 00     0.90167E 00     0.11270E 01     0.20416E 01     0.96735E 00     0.27934E-05     0.19015E-05     0.33164E-04
                0.28248E-04     0.20000E 03

     460.00     0.84734E 00     0.90167E 00     0.11270E 01     0.20416E 01     0.96735E 00     0.27934E-05     0.19015E-05     0.33164E-04
                0.28248E-04     0.20000E 03
                     NUMBER OF TIME STEPS IN CYCLE NO.      1  IS    65    DIFFERENTIAL CP TIME =      0.0   SEC
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS          CP TIME =    0.000DATE       QTO-  PAGE   15



                         CONCENTRATION PROFILES-PARTS PER HUNDRED MILLION

                                       TIME= 0.60000E 02 MINUTES

     GROUND DIFFUSIVITY =  59.999954                  K1 = 0.43750000
 NO   FLUX =     0.0
 HC   FLUX =     0.0
 CO   FLUX =     0.0

HEIGHT-M.   NO            HC             NO2            OZON           HNO2           NO3            N2O5           OH
              RO2            CO

  0.0      0.75635E 00   0.81447E 00    0.11928E 01    0.25059E 01    0.93295E 00    0.34287E-05    0.24704E-05    0.32484E-04
           0.28009E-04   0.20001E 03

115.00     0.75635E 00   0.81447E 00    0.11928E 01    0.25059E 01    0.93295E 00    0.34287E-05    0.24704E-05    0.32484E-04
           0.23009E-04   0.20000E 03

230.00     0.75635E 00   0.81447E 00    0.11928E 01    0.25059E 01    0.93295E 00    0.34287E-05    0.24704E-05    0.32484E-04
           0.28009E-04   0.20000E 03

345.00     0.75635E 00   0.81447E 00    0.11928E 01    0.25059E 01    0.93295E 00    0.34287E-05    0.24704E-05    0.32484E-04
           0.28009E-04   0.20000E 03

460.00     0.75635E 00   0.81447E 00    0.11928E 01    0.25059E 01    0.93295E 00    0.34287E-05    0.24704E-05    0.32484E-04
           0.28009E-04   0.20001E 03

       ---      NUMBER OF TIME STEPS IN CYCLE NO.      2  IS   60    DIFFERENTIAL CP TIME =      0.0   SEC
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS              CP TIME =    0.000ATE       QTD-  PAGE   16




                                CONCENTRATION PROFILES-PARTS PER HUNDRED MILLION

                                          TIME= 0.90000E 02 MINUTES

      GROUND DIFFUSIVITY =  59.999954                     K1 = 0.44664997
 NO    FLUX =     0.0
 HC    FLUX =     0.0
 CO    FLUX =     0.0

HEIGHT-M.   NO              HC              NO2             OZON            HNO2            NO3             N2O5            OH
              RO2             CO

   0.0      0.68765E 00     0.73691E 00     0.12341E 01     0.29251E 01     0.89778E 00     0.40022E-05     0.29835E-05     0.31784E-04
            0.27281E-04     0.20001E 03

 115.00     0.68764E 00     0.73691E 00     0.12341E 01     0.29251E 01     0.89778E 00     0.40022E-05     0.29835E-05     0.31784E-04
            0.27281E-04     0.20000E 03

 230.00     0.68764E 00     0.73691E 00     0.12341E 01     0.29251E 01     0.89778E 00     0.40022E-05     0.29835E-05     0.31784E-04
            0.27281E-04     0.20000E 03

 345.00     0.68764E 00     0.73691E 00     0.12341E 01     0.29251E 01     0.89778E 00     0.40022E-05     0.29835E-05     0.31784E-04
            0.27281E-04     0.20000E 03

 460.00     0.68764E 00     0.73691E 00     0.12341E 01     0.29251E 01     0.89778E 00     0.40022E-05     0.29835E-05     0.31784E-04
            0.27281E-04     0.20001E 03
                    NUMBER OF TIME STEPS IN CYCLE NO.      3  IS   60    DIFFERENTIAL CP TIME =     0.0   SEC
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS            CP TIME =    0.00DATE       QTO-  PAGE   17



                              CONCENTRATION PROFILES-PARTS PER HUNDRED MILLION

                                        TIME= 0.12000E 03 MINUTES
         GROUND DIFFUSIVITY =  59.999954                      KI = 0.45164996
   NO    FLUX =    0.50837919E-02
   HC    FLUX =      1.5594149
   CO    FLUX =      1.2712097

HEIGHT-M.  NO              HC
             RO2             CO           NO2          OZON          HNO2          NO3           N2O5          OH

   0.0     0.62734E 00   0.83613E 00   0.12690E 01   0.33266E 01   0.86255E 00   0.45515E-05   0.34886E-05   0.30814E-04
           0.32906E-04   0.20067E 03
 115.00    0.63031E 00   0.72422E 00   0.12637E 01   0.33097E 01   0.86257E 00   0.45285E-05   0.34566E-05   0.30877E-04
           0.28426E-04   0.20030E 03
 230.00    0.63166E 00   0.68303E 00   0.12610E 01   0.33005E 01   0.86257E 00   0.45158E-05   0.34396E-05   0.30913E-04
           0.26782E-04   0.20010E 03
 345.00    0.63206E 00   0.67140E 00   0.12601E 01   0.32975E 01   0.86258E 00   0.45118E-05   0.34342E-05   0.30925E-04
           0.26320E-04   0.20003E 03
 460.00    0.63214E 00   0.66924E 00   0.12600E 01   0.32970E 01   0.86258E 00   0.45110E-05   0.34331E-05   0.30927E-04
           0.26234E-04   0.20001E 03
                NUMBER OF TIME STEPS IN CYCLE NO.      4  IS   60   DIFFERENTIAL CP TIME =      0.0   SEC
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS              CP TIME =    0.00DATE       QTO-  PAGE   18



                                CONCENTRATION PROFILES-PARTS PER HUNDRED MILLION

                                             TIME= 0.15000E 03 MINUTES

      GROUND DIFFUSIVITY =  59.999954                     K1 = 0.45163995
   NO   FLUX =     0.35061002
   HC   FLUX =      14.734360
   CO   FLUX =      28.581619

  HEIGHT-M.   NO             HC              NO2             OZON            HNO2            NO3             N2O5            OH
                RO2            CO

    0.0       0.64058E 00    0.24164E 01     0.14962E 01     0.37330E 01     0.82786E 00     0.51076E-05     0.46159E-05     0.26015E-04
              0.78723E-04    0.20625E 03

  115.00      0.59184E 00    0.11546E 01     0.13448E 01     0.37065E 01     0.82786E 00     0.50714E-05     0.41195E-05     0.28593E-04
              0.44720E-04    0.20213E 03

  230.00      0.58096E 00    0.74265E 00     0.12907E 01     0.36683E 01     0.82789E 00     0.50191E-05     0.39130E-05     0.29612E-04
              0.30341E-04    0.20071E 03

  345.00      0.58070E 00    0.64345E 00     0.12782E 01     0.36467E 01     0.82792E 00     0.49896E-05     0.38524E-05     0.29838E-04
              0.26499E-04    0.20025E 03

  460.00      0.58110E 00    0.62578E 00     0.12761E 01     0.36403E 01     0.82793E 00     0.49808E-05     0.38392E-05     0.29873E-04
              0.25784E-04    0.20014E 03

                 NUMBER OF TIME STEPS IN CYCLE NO.       5  IS  103    DIFFERENTIAL CP TIME =      0.0   SEC
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS             CP TIME =    0.000ATE       QTO-  PAGE    19




                          CONCENTRATION PROFILES-PARTS PER HUNDRED MILLION

                                          TIME= 0.18000E 03 MINUTES

       GROUND DIFFUSIVITY =  59.999954                  K1 = 0.44663996
   NO   FLUX =     0.27539515
   HC   FLUX =      2.4632092
   CO   FLUX =      40.547745

 HEIGHT-M.   NO               HC               NO2              OZON             HNO2             NO3              N2O5             OH
              RO2              CO

   0.0      0.52126E 00     0.25446E 01     0.15562E 01     0.47024E 01     0.79368E 00     0.64340E-05     0.60479E-05     0.24795E-04
            0.97199E-04     0.21506E 03

 115.00     0.51724E 00     0.17889E 01     0.14564E 01     0.44814E 01     0.79384E 00     0.61315E-05     0.53941E-05     0.26098E-04
            0.72438E-04     0.20682E 03

 230.00     0.52398E 00     0.11563E 01     0.13702E 01     0.42264E 01     0.79405E 00     0.57827E-05     0.47860E-05     0.27302E-04
            0.48332E-04     0.20292E 03

 345.00     0.53024E 00     0.82173E 00     0.13222E 01     0.40682E 01     0.79420E 00     0.55662E-05     0.44454E-05     0.28019E-04
            0.34823E-04     0.20127E 03

 460.00     0.53255E 00     0.72470E 00     0.13079E 01     0.40183E 01     0.79425E 00     0.54979E-05     0.43434E-05     0.28238E-04
            0.30814E-04     0.20083E 03

                     NUMBER OF TIME STEPS IN CYCLE NO.      6  IS    60    DIFFERENTIAL CP TIME =      0.0   SEC
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS              CP TIME =    0.00DATE       QTO-  PAGE   20




                                 CONCENTRATION PROFILES-PARTS PER HUNDRED MILLION

                                           TIME= 0.21000E 03 MINUTES

     GROUND DIFFUSIVITY =  59.999954                  K1 = 0.43748999
 NO   FLUX =     0.15759951
 HC   FLUX =       1.4531088
 CO   FLUX =      19.533218

HEIGHT-M.   NO              HC             NO2            OZON           HNO2           NO3            N2O5           OH
              RO2             CO

  0.0      0.44384E 00    0.24988E 01    0.15886E 01    0.55310E )1    0.76067E 00    0.75676E-05    0.72616E-05    0.23475E-04
           0.10624E-03    0.21299E 03

115.00     0.44660E 00    0.19291E 01    0.15140E 01    0.52822E 01    0.76089E 00    0.72273E-05    0.66095E-0:    0.24310E-04
           0.84371E-04    0.20842E 03

230.00     0.45850E 00    0.13915E 01    0.14377E 01    0.49448E 01    0.76123E 00    0.67655E-05    0.58752E-05    0.25206E-04
           0.61428E-04    0.20518E 03

345.00     0.46969E 00    0.10566E 01    0.13848E 01    0.46882E 01    0.76152E 00    0.64145E-05    0.53655E-05    0.25870E-04
           0.46714E-04    0.20316E 03

460.00     0.47414E 00    0.94583E 00    0.13662E 01    0.45952E 01    0.76163E 00    0.62873E-05    0.51884E-05    0.26113E-04
           0.41808E-04    0.20249E 03

                 NUMBER OF TIME STEPS IN CYCLE NO.     7  IS   60    DIFFERENTIAL CP TIME =     0.0   SEC
```

```
DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS                CP TIME =     0.00DATE       QTO-  PAGE   21




                                          CONCENTRATION PROFILES-PARTS PER HUNDRED MILLION

                                                    TIME= 0.24000E 03 MINUTES

      GROUND DIFFUSIVITY =  59.999954                            K1 = 0.42534000
 NO   FLUX =      0.15759951
 HC   FLUX =       1.4531088
 CO   FLUX =      19.533218

HEIGHT-M.   NO              HC                 NO2             OZON           HNO2           NO3            N2O5           OH
             RO2             CO

   0.0     0.39231E 00    0.20482E 01     0.15884E 01    0.61602E 01    0.72929E 00    0.84286E-05    0.80866E-05    0.22213E-04
           0.93337E-04    0.21597E 03

 115.00    0.39214E 00    0.17588E 01     0.15360E 01    0.59718E 01    0.72949E 00    0.81708E-05    0.75810E-05    0.22789E-04
           0.82222E-04    0.21066E 03

 230.00    0.40077E 00    0.14491E 01     0.14810E 01    0.56695E 01    0.72983E 00    0.77572E-05    0.69394E-05    0.23383E-04
           0.67975E-04    0.20707E 03

 345.00    0.41024E 00    0.12184E 01     0.14396E 01    0.54120E 01    0.73014E 00    0.74048E-05    0.64388E-05    0.23842E-04
           0.56904E-04    0.20500E 03

 460.00    0.41425E 00    0.11341E 01     0.14242E 01    0.53130E 01    0.73026E 00    0.72693E-05    0.62534E-05    0.24016E-04
           0.52830E-04    0.20432E 03

                 NUMBER OF TIME STEPS IN CYCLE NO.      8   IS   60   DIFFERENTIAL CP TIME =      0.0   SEC


DIFKIN SAMPLE RUN - COMPUTE TRAJECTORY, FLUXES, AND CONCENTRATIONS                      CP TIME =     0.00DATE
                 NUMBER OF TIME STEPS =      528          CP TIME =      60.00   SEC
```